NYO-1480-75

Courant Institute of
Mathematical Sciences

AEC Computing and Applied Mathematics Center

# The One Body Wigner-Moyal Density for a Locally Linear Potential of Arbitrary Dimension

Jerome K. Percus and John Snygg

AEC Research and Development Report

Physics
June 1967

New York University

NEW YORK UNIVERSITY
COURANT INSTITUTE - LIBRARY
251 Mercer St. New York, N.Y. 10012

UNCLASSIFIED

AEC Computing and Applied Mathematics Center
Courant Institute of Mathematical Sciences
New York University

Physics NYO-1480-75

# THE ONE BODY WIGNER-MOYAL DENSITY FOR A LOCALLY LINEAR POTENTIAL OF ARBITRARY DIMENSION

Jerome K. Percus and John Snygg

Contract No. AT(30-1)-1480

UNCLASSIFIED

NEW YORK UNIVERS
COURANT INSTITUTE - LI

C.1

# Contents

Page

Introduction 1

## Part I

Section 1. Generalized Remarks 3

The one body Dirac density for a non-interacting many body system is written down in terms of an operator acting on the Dirac delta function and also in terms of an operator integral.

Section 2. Zero Order Approximation 5

The Thomas Fermi approximation is extracted from the operator integral introduced in Sec. 1.

Section 3. The N Particle Wigner-Moyal Density for D Dimension 7

The one body Wigner-Moyal density for a non-interacting system of N particles is written down in terms of an operator acting on 1.

Section 4. Expansion of Wigner-Moyal Density in Powers of $\hbar$. 9

The results of Kompaneets and Pavlovskii, Kirzhnits, Golden, Baraff and Borowitz are briefly reviewed in relation to the Wigner-Moyal density.

Section 5. W.K.B.-Like Approximation 11

Making the approximation of a locally linear potential or slowly varying force field the operator acting on 1 (Section 3) is explicitly computed and written down in terms of an integral (p. 15). From this integral the space and kinetic energy densities are computed (p. 16). The Wigner-Moyal space and kinetic energy densities are

Page

rewritten in other forms (p. 17-19). Asymptotic forms are written down for the 3 dimensional case (p. 20) and for the 1 dimensional case (p. 21). The 1 dimensional asymptotic expansion is compared with a result of Kohn and Sham (p. 21-22).

Section 6. Relation to W.K.B. Method 23

Section 7. Region Near Nucleus of an Atom 25

Section 8. Bohr Sommerfeld Rule for Hydrogen Atom 29

Part II

Section 1. Exact Wigner-Moyal Density for Non-Interacting Harmonic Oscillator. 31

Exact densities for the harmonic oscillator are computed and compared with the approximate densities obtained in Section 3 of Part I.

Section 2. Dirac Density for Harmonic Oscillator with $D = 2k+1$. 43

Section 3. The Interacting Harmonic Oscillator 46

The exact densities are computed for the interacting harmonic oscillator with a "closed shell" structure.

Section 4. The Hartree-Fock Solution Minus the Exchange Term for the D Dimensional, $N_p$ Particle Interacting Harmonic Oscillator. 60

Section 5. The Thomas Fermi Approximation for the Interacting Harmonic Oscillator 63

Page

## Appendices

Appendix 1. 68

The Wigner-Moyal density is discussed in general terms (p. 68-74). The solutions for the free particle minimum wave packet and the harmonic oscillator are computed and discussed (p. 74-78). The Kirkwood density is discussed (p. 79-81) and the relation between the Wigner-Moyal and Kirkwood densities is written down (p. 82).

Appendix 2. 83

A necessary approximate commutation relation is developed.

Appendix 3. 86

It is shown how certain Airy function integrals may be written explicitly in terms of the Airy function and a finite number of its derivatives.

Appendix 4. 90

The asymptotic expansions for $\rho(\underset{\sim}{r})$ and $t(\underset{\sim}{r})$ are computed.

References 103

# ABSTRACT

Using the Wigner-Moyal density and operator techniques, W.K.B. like solutions are obtained in closed form for a system of non-interacting particles in an arbitrary potential of arbitrary dimension. For three dimensions the first three terms of the asymptotic expansion give the Thomas Fermi approximation with the Weizsäcker correction reduced by 1/9 plus an oscillatory term of amplitude 6 times the reduced Weizsäcker correction. For one dimension the first two terms correspond to a result of Kohn and Sham.

# Introduction

In the late twenties when the Thomas-Fermi model for atom was first introduced, it was recognized as being crude.

During the early thirties various ad hoc corrections were attempted. Of these the most prominent were the Dirac exchange term due to P. A. M. Dirac [1] and the Weizsacker term due to C. F. van Weizsäcker [2].

At the same time the Hartree and Hartree-Fock approximations emerged. These approximations give highly satisfactory results, but the computations are lengthy and only feasible for atoms, ions, or molecules either with a very small number of electrons or with a small number of electrons in a highly symmetric set of orbits.

However the success of the Hartree and Hartree-Fock approximations led people to seek some understanding of the connection between those approximations and that of the Thomas-Fermi model.

In 1957 in the work of A. S. Kompaneets and E. S. Pavlovskii [3], D. A. Kirzhnits [4], and S. Golden [5] it was shown that if one expanded the diagonal part of the Hartree-Fock density matrix in increasing powers of $\hbar$ that the zero order term was the Thomas-Fermi result. Proceeding along this way the same men found that the first correction to that (the $\hbar^2$ term) gives the Weizsäcker term reduced by 1/9 plus the Dirac exchange term.

However the resulting computations were unsatisfactory and it was observed that this approach would never give the oscillatory behavior corresponding to the shell structure of Hartree and Hartree-Fock solutions.

More recently Von W. Macke and P. Rennert [6] using operator techniques and W. Kohn and L. J. Sham [7] using Green's functions have successfully remedied this last problem for one dimension with very encouraging results.

In this paper we will show how formulating the required equations in terms of the Wigner-Moyal density makes it possible to generalize the one dimensional results of Von W. Macke and P. Rennert to D dimensions. Since our approximations break down near $r = 0$ for a Coulomb potential, we will also discuss boundary conditions at that point.

# Part I

## Section 1. Generalized Remarks.

In a paper published in 1963, W. Macke and P. Rennert [6] following a technique of D. A. Kiŕzhnits [4] and S. Golden [5] were able to write down the Dirac density in terms of an operator integral for a many body system in which all particles experience the same potential.

From this integral, Macke and Rennert showed that the Thomas-Fermi solution dropped out as a zero order approximation in the D dimensional case. And then restricting themselves to potentials either one dimensional or radially symmetric, they were able to get W. K. B. like solutions as first order approximations.

In this paper, we will show how the results of Macke and Rennert can be generalized to the case of a general D dimensional potential.

It is hoped that our results will make it practicable to get satisfactory computations for binding energies of heavy molecules.

We now begin in the same fashion as Macke and Rennert.

For a system of N = 2A independent particles in a common D dimensional potential, we have:

$$(I.1.1) \qquad \hat{H}(\underset{\sim}{r})\ \psi_n(\underset{\sim}{r}) = E_n\ \psi_n(\underset{\sim}{r})$$

where

$$\hat{H}(\underset{\sim}{r}) = \frac{\hat{\underset{\sim}{p}}^{2}}{2m} + V(\underset{\sim}{r}) = \frac{-\hbar^{2}}{2m} \sum_{i=1}^{D} \frac{\partial^{2}}{\partial x^{2}} + V(\underset{\sim}{r}) .$$

The Dirac density for the lowest energy state is:

$$\text{(I.1.2)} \qquad \rho(\underset{\sim}{r},\underset{\sim}{r}') = 2 \sum_{n=1}^{A=N/2} \psi_n(\underset{\sim}{r})\, \psi_n^{*}(\underset{\sim}{r}') .$$

The factor 2 was inserted above to take care of spin.

Since the $\psi_n(\underset{\sim}{r})$ form a complete system

$$\text{(I.1.3)} \qquad \sum_{n=1}^{\infty} \psi_n(\underset{\sim}{r})\, \psi_n^{*}(r') = \delta(\underset{\sim}{r}-\underset{\sim}{r}') .$$

We can now rewrite (I.1.2) in the form:

$$\text{(I.1.4)} \quad \rho(\underset{\sim}{r},\underset{\sim}{r}') = 2 \sum_{n=1}^{\infty} \theta(A^{+}-n)\, \psi_n(\underset{\sim}{r})\, \psi_n^{*}(\underset{\sim}{r}')$$

where

$$\theta(\alpha) = \begin{cases} 1 & \text{if } \alpha > 0 \\ 1/2 & \alpha = 0 \\ 0 & \alpha < 0 \end{cases}$$

and

$$A < A^{+} < A + 1$$

If we assume $\rho(\underset{\sim}{r},\underset{\sim}{r}')$ is composed of the lowest energy levels and $E_A < E_{A+1}$ then:

$$\text{(I.1.5)} \quad \rho(\underset{\sim}{r},\underset{\sim}{r}') = 2 \sum_{n=1}^{\infty} \theta(E-E_n)\, \psi_n(\underset{\sim}{r})\, \psi_n^{*}(\underset{\sim}{r}')$$

where $E_A < E < E_{A+1}$.

But

$$f(\hat{H})\ \psi_n(\underset{\sim}{r}) = f(E_n)\ \psi_n(\underset{\sim}{r})$$

so

$$(\text{I.1.6})\qquad \rho(\underset{\sim}{r},\underset{\sim}{r}') = 2\sum_{n=1}^{\infty}\Theta(E-\hat{H})\psi_n(\underset{\sim}{r})\psi_n^*(\underset{\sim}{r}') = 2\Theta(E-\hat{H})\delta(\underset{\sim}{r}-\underset{\sim}{r}')\ .$$

Now we may write:

$$(\text{I.1.7})\qquad \Theta(\alpha) = \frac{-1}{2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{e^{-i\alpha\omega}}{\omega}\,d\omega\ ,$$

and

$$(\text{I.1.8})\qquad \delta(\underset{\sim}{r}-\underset{\sim}{r}') = \frac{1}{h^D}\iint e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}}\,d\underset{\sim}{p}\ ,$$

where $h = 2\pi\hbar$.

Combining (I.1.6), (I.1.7) and (I.1.8) we get:

$$(\text{I.1.9})\qquad \rho(r,r') = \frac{-2}{h^D 2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{e^{-i\omega(E-\hat{H})}}{\omega}d\omega\iint e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}}\,d\underset{\sim}{p}\ .$$

## Section 2. Zero Order Approximation.

Macke and Rennert pointed out that to get the zero order approximation we assume that:

$$(\text{I.2.1})\qquad T = \frac{-\hbar^2}{2m}\sum_{i=1}^{D}\frac{\partial^2}{\partial x_i^2}\quad \text{and}\quad V(\underset{\sim}{r})\quad \text{commute.}$$

From (I.1.6) and (I.1.8) we get:

$$(I.2.2) \qquad \rho(\underset{\sim}{r},\underset{\sim}{r}') = \frac{2}{h^D} \iint \Theta(E-\hat{H}(\hat{\underset{\sim}{p}},\hat{\underset{\sim}{r}}))\, e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{h}}\, d\underset{\sim}{p} \ .$$

Now using approximation (I.2.1) and then setting $\underset{\sim}{r}' = \underset{\sim}{r}$, we get the zero order approximation for the space density $\rho(\underset{\sim}{r})$.

$$(I.2.3) \qquad \rho(\underset{\sim}{r}) = \frac{2\Omega_D}{h^D} \int_0^\infty \Theta(E - V(\underset{\sim}{r}) - \frac{p^2}{2m})\, p^{D-1}\, dp$$

where

$$(I.2.4) \qquad \begin{aligned} \Omega_1 &= 2 \\ \Omega_2 &= 2\pi \\ \Omega_3 &= 4\pi \quad \text{and in general} \\ \Omega_D &= 2\pi^{D/2}/\Gamma(D/2) \ . \end{aligned}$$

Integrating (I.2.3) we have:

$$(I.2.5) \qquad \rho(\underset{\sim}{r}) = \begin{cases} \dfrac{2\Omega_D}{h^D \cdot D}\,[2m(E-V(\underset{\sim}{r}))]^{D/2} & \text{if } E > V(\underset{\sim}{r}) \ ; \\ 0 & \text{if } E < V(\underset{\sim}{r}) \ . \end{cases}$$

For the case D = 3, (I.2.5) is precisely the Thomas Fermi or T.F. approximation. One only needs to add the requirement that $\nabla^2 V = -4\pi e^2 \rho(\underset{\sim}{r})$ to get the usual equation for the potential of the T.F. atom [8].

## Section 3. The N Particle Wigner-Moyal Density for D Dimensions.

We shall begin by rewriting equation (I.2.2)

$$(I.2.2)\quad \rho(\underset{\sim}{r},\underset{\sim}{r}') = \frac{2}{h^D} \iint \theta(E-\hat{H}(\hat{\underset{\sim}{p}},\hat{\underset{\sim}{r}}))\, e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}}\, d\underset{\sim}{p}$$

but

$$(I.3.1)\quad \theta(E-\hat{H})e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}}$$

$$= \iint d\underset{\sim}{r}''\delta(\underset{\sim}{r}-\underset{\sim}{r}'')\ \theta(E-\sum_{i=1}^{D}\frac{(\hat{p}_i+\hat{p}_i'')^2}{2m} - V(\underset{\sim}{r}''))\ e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}}$$

where:

$\hat{p}_i$ acts only on $f(\underset{\sim}{r})$ (in this case $e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}/\hbar}$),

$\hat{p}_i''$ acts only on $f(\underset{\sim}{r}'')$ (in this case $V(\underset{\sim}{r}'')$, and

$p_i$ is the i-th component of $\underset{\sim}{p}$.

Now it is clear we may replace the operator $\hat{p}_i$ in (I.3.1) by the corresponding scalar $p_i$, giving us the equation:

$$(I.3.2)\quad \theta(E-\hat{H})e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}}$$

$$= \iint d\underset{\sim}{r}''\delta(\underset{\sim}{r}-\underset{\sim}{r}'')\ \theta(E-\sum_{i=1}^{D}\frac{(p_i+\hat{p}_i'')^2}{2m} - V(\underset{\sim}{r}''))\ e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}}$$

or after integrating:

$$(\text{I.3.3})\quad \theta(E-\hat{H})\, e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}} = e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{\hbar}}\, \theta(E-\sum_{i=1}^{D}\frac{(p_i+\hat{p}_i)}{2m}-V(\underset{\sim}{r}))\cdot 1.$$

Thus (I.2.2) may be rewritten in the form

$$(\text{I.3.4})\quad \rho(\underset{\sim}{r},\underset{\sim}{r}') = \iint d\underset{\sim}{p}\; e^{\frac{i\underset{\sim}{p}\cdot(\underset{\sim}{r}-\underset{\sim}{r}')}{h}}\; \frac{2}{h^D}\,\theta(E-\sum_{i=1}^{D}\frac{(p_i+\hat{p}_i)}{2m}-V(\underset{\sim}{r}))\cdot 1.$$

Now from equation (A.1.34) in Appendix 1 it is clear we now have a formula for the complex conjugate of the Kirkwood density,

$$(\text{I.3.5})\qquad \rho_k^*(\underset{\sim}{p},\underset{\sim}{r}) = \frac{2}{h^D}\,\theta(E-\sum_{i=1}^{D}\frac{(p_i+\hat{p}_i)^2}{2m}-V(r))\cdot 1$$

Using equation (A.1.38) and keeping in mind that the Wigner-Moyal density is real we get a formula for Wigner-Moyal density,

$$(\text{I.3.6})\qquad \rho(\underset{\sim}{p},\underset{\sim}{r}) = \exp\left(\frac{i\hbar}{2}\sum_{i=1}^{D}\frac{\partial^2}{\partial p_i\,\partial x_i}\right)\rho_k^*(\underset{\sim}{p},\underset{\sim}{r})$$

and now from (I.3.5) noting that $\frac{\hbar}{i}\frac{d}{dx_i} = \hat{p}_i$ ,

$$\boxed{(\text{I.3.7})\quad \rho(\underset{\sim}{p},\underset{\sim}{r}) = \exp\left(-\frac{1}{2}\sum_{i=1}^{D}\hat{p}_i\frac{d}{dp_i}\right)\left[\frac{2}{h^D}\,\theta(E-\sum_{i=1}^{D}\frac{(p_i+\hat{p}_i)^2}{2m}-V(\underset{\sim}{r}))\cdot 1\right]}$$

If we were to make the T.F. approximation that

$dV(\underset{\sim}{r})/dx_i \approx 0$ i.e. $V(\underset{\sim}{r}) \approx$ a constant, then (I.3.7) becomes

$$\text{(I.3.8)} \qquad \rho(\underset{\sim}{p},\underset{\sim}{r}) \approx \frac{2}{h^D}\,\Theta(E - H(\underset{\sim}{p},\underset{\sim}{r})) \;.$$

## Section 4. Expansion of Wigner-Moyal Density in Powers of ħ.

One way to extract something useful out of (I.3.7) is to expand $\rho(\underset{\sim}{p},\underset{\sim}{r})$ in increasing powers of h, keeping in mind that $\hat{p}_i = \frac{\hbar}{i}\frac{d}{dx_i}$ .

Doing this we get:

$$\text{(I.4.1)} \quad \frac{h^D}{2}\,\rho(\underset{\sim}{p},\underset{\sim}{r}) = \Theta(E - H)$$

$$+ \frac{\hbar^2}{24m}\Big[\sum_{i=1}^{D}\Big(\frac{\partial V}{\partial x_i}\Big)^2 \Theta^{(3)}(E-H) + 2\sum_{i,j}^{D}\Big(\frac{\partial^2 V}{\partial x_i \partial x_j}\Big)\frac{p_i p_j}{2m}\,\Theta^{(3)}(E-H)$$

$$- 3\sum_{i=1}^{D}\Big(\frac{\partial^2 V}{\partial x_i^2}\Big)\Theta^{(2)}(E - H)\Big] + O(\hbar^4) \;,$$

where $H = \sum_{i=1}^{D}\frac{p_i^2}{2m} + V(\underset{\sim}{r})$.

If we ignore the second order derivatives and integrate out momentum we get the space density

$$\text{(I.4.2)} \quad \rho(\underset{\sim}{r}) = \begin{cases} \dfrac{2\Omega_D[2m(E-V(\underset{\sim}{r}))]^{D/2}}{h^D\,D}\Big[1+\dfrac{D\cdot(D-2)(D-4)}{24}\,\dfrac{m^2\hbar^2|\underset{\sim}{\nabla}V|^2}{[2m(E-V(\underset{\sim}{r}))]^3}\Big], & E > V \\ 0 \;, & E < V \end{cases}$$

In 1957, Kompaneets and Pavlovskii [3] were the first to compute a similar series for $\rho(\underset{\sim}{r})$ in powers of $\hbar$. However their method involved using a system of hierarchy equations with non-unique solutions.

Shortly afterward in the same year D. A. Kirzhnits [4] was able to apply some operator techniques he developed to put such a series for $\rho(\underset{\sim}{r})$ on a sounder footing.

Although D. A. Kirzhnits wrote down the first few terms for $\rho(\underset{\sim}{r})$ and not for the more useful Wigner-Moyal density $\rho(\underset{\sim}{p},\underset{\sim}{r})$, he was still able to use his methods to compute any expectation value. At any rate it is only a short step from his work to equation (I.4.1) and we have used methods very similar to his to get it.

In 1960, G. A. Baraff and S. Borowitz [9] developed a very clean method for getting a similar expansion for the Green's function corresponding to the Wigner-Moyal density.

The first term in (I.4.1) is of course the Thomas Fermi approximation. The first term of order $\hbar^2$ in the square brackets is the source of the second term in (I.4.2) which is generally referred to as the Weizsäcker correction.1/

Kompaneets and Pavlovskii pointed out that the Dirac-exchange term is also of order $\hbar^2$ and should be

---

1/ Our "Weizsäcker" term is that of Kompaneets and Pavlovskii i.e. 1/9 of the original one.

treated as a correction to the T.F. approximation of the same order as the Weizsäcker term.

One could continue expanding $\rho(\underset{\sim}{p},\underset{\sim}{r})$ out further in this fashion. However all correction terms are functions of the $p_i$'s and derivatives of $V(\underset{\sim}{r})$ multiplied by higher order derivatives of $\Theta(E-H)$ which are in turn derivatives of $\delta(E-H)$. So it is clear that additional terms may possibly improve some expectation values but they certainly will not affect the actual Wigner-Moyal density away from the point where $H = E$. Thus it is clear that not all expectation values would be improved.

Having discussed the power series approach, let us return to (I.3.7) and try a hopefully more fruitful method.

## Section 5. W.K.B.-like Approximation: $\partial^2 V/\partial x_i \partial x_j = 0$.

From (I.1.7) we may write

$$\text{(I.5.1)}\quad \Theta\Big(E-\sum_{i=1}^{D}\frac{(p_i+\hat{p}_i)^2}{2m}-V(\underset{\sim}{r})\Big)$$

$$= -\frac{1}{2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{d\omega}{\omega}\, e^{-i\omega(E-\sum_{i=1}^{D}\frac{p_i^2}{2m})}\, e^{i\omega(\sum_{i=1}^{D}\frac{\hat{p}_i^2+2p_i\hat{p}_i}{2m}+V(\underset{\sim}{r}))}\ .$$

Now let us consider the operator

$$(\text{I.5.2}) \qquad e^{A+B} = e^{i\omega\left(\sum_{i=1}^{D} \frac{\hat{p}_i^2+2p_i\hat{p}_i}{2m} + V(\underset{\sim}{r})\right)}$$

where

$$(\text{I.5.3}) \begin{cases} A = i\omega\, V(\underset{\sim}{r}) \\ B = i\omega \sum_{i=1}^{D} \left(\frac{\hat{p}_i^2+2p_i\hat{p}_i}{2m}\right) = -\frac{i\omega}{2m} \sum_{i=1}^{D} \left(\hbar^2 \frac{\partial^2}{\partial x_i^2} + 2i\hbar p_i \frac{\partial}{\partial x_i}\right) \end{cases}$$

$$(\text{I.5.4}) \begin{cases} [B,A] = \frac{\omega^2}{2m} \left[\hbar^2\left( \sum_{i=1}^{D} \frac{\partial^2 V}{\partial x_i^2} + 2 \sum_{i=1}^{D} \frac{\partial V}{\partial x_i} \frac{\partial}{\partial x_i}\right) + 2i\hbar \sum_{i=1}^{D} p_i \frac{\partial V}{\partial x_i}\right] \\ [[B,A],A] = \frac{i\omega^3\hbar^2}{m} \sum_{i=1}^{D} \left(\frac{\partial V}{\partial x_i}\right)^2 \\ [[[B,A],A],A] = 0 \end{cases}$$

Now we make the approximation that B, [B,A], and [[B,A],A] commute with one another. Doing this and using equation (A.2.12), we get

$$(\text{I.5.5}) \qquad e^{A+B} = e^A \cdot e^{(B+ \frac{1}{2}[B,A]+ \frac{1}{6}[[B,A],A])}$$

This approximation corresponds to assuming $\partial^2 V/\partial x_i \partial x_j = 0$.

We should note that in comparing this approach to that used in the last section, we are in effect ignoring the second and third terms of order $\hbar^2$ in the square brackets of equation (I.4.1).

However these terms are usually ignored anyway and we are no longer making the approximation that $\hbar$ is near zero.

Collecting (I.5.2), (I.5.4) and (I.5.5) together we have:

$$(\text{I.5.6})\quad e^{i\omega\left(\sum_{i=1}^{D}\frac{\hat{p}_i^2+2p_i\hat{p}_i}{2m}+V(\underset{\sim}{r})\right)}\cdot 1 = e^{\left[i\omega V(\underset{\sim}{r})+\frac{i\omega^2\hbar}{2m}\sum_{i=1}^{D}p_i\frac{\partial V(\underset{\sim}{r})}{\partial x_i}+\frac{i\omega^3\hbar^2}{6m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2\right]}$$

From (I.3.7), (I.5.1), and (I.5.6) we get

$$(\text{I.5.7})\quad \rho(\underset{\sim}{p},\underset{\sim}{r}) = -\frac{2}{h^D}\frac{i}{2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{d\omega}{\omega}\,e^{-i\omega E}\,e^{-\frac{1}{2}\sum_{i=1}^{D}\hat{p}_i\frac{\partial}{\partial p_i}}\cdot e^{\left(i\omega H+\frac{i\omega^2\hbar}{2m}\sum_{i=1}^{D}p_i\frac{\partial V}{\partial x_i}+\frac{i\omega^3\hbar^2}{6m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2\right)}.$$

Keeping in mind the approximation that $\partial^2V/\partial x_i\partial x_j = 0$, it can be shown by induction on N that

$$(\text{I.5.8}) \quad \left( -\frac{1}{2}\sum_{i=1}^{D} \hat{p}_i \frac{\partial}{\partial p_i} \right)^N \exp\left(i\omega H(\underset{\sim}{p},\underset{\sim}{r}) + \frac{i\omega^2\hbar}{2m}\sum_{i=1}^{D} p_i \frac{\partial V}{\partial x_i} + \frac{i\omega^3\hbar^2}{6m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2\right)$$

$$= \sum_{k=0}^{[N/2]} \frac{N!\,(-1)^N}{(N-2k)!\,k!}\, u^{N-2k}\, v^k \exp\left(i\omega H + \frac{i\omega^2\hbar}{2m}\sum_{i=1}^{D} p_i \frac{\partial V}{\partial x_i} + \frac{i\omega^3\hbar^2}{6m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2\right)$$

where $[N/2]$ is the greatest integer $\leq N/2$, and

$$(\text{I.5.9}) \quad \begin{aligned} u &= \frac{i\hbar\omega^2}{2m}\sum_{i=1}^{D} p_i \frac{\partial V}{\partial x_i} + \frac{i\omega^3\hbar^2}{4m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2 \\ v &= \frac{i\omega^3\hbar^2}{8m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2 \end{aligned}$$

Noting that

$$(\text{I.5.10}) \quad e^{-\frac{1}{2}\sum_{i=1}^{D} \hat{p}\cdot \frac{\partial}{\partial p_i}} = \sum_{N=0}^{\infty} \frac{\left(-\frac{1}{2}\sum_{i=1}^{D} \hat{p}_i \frac{\partial}{\partial p_i}\right)^N}{N!}$$

and

$$(\text{I.5.11}) \quad \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{k=0}^{[N/2]} \frac{N!\,(-1)^N}{(N-2k)!\,k!}\, u^{N-2k}\, v^k$$

$$= \sum_{k=0}^{\infty} \frac{v^k}{k!} \sum_{N=2k}^{\infty} \frac{(-1)^N}{(N-2k)!}\, u^{N-2k}$$

$$= e^{v-u} = \exp\left[ -\frac{i\hbar\omega^2}{2m}\sum_{i=1}^{D} p_i \frac{\partial V}{\partial x_i} - \frac{i\omega^3\hbar^2}{8m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2\right].$$

We conclude that

$$e^{-\frac{1}{2}\sum_{i=1}^{D}\hat{p}_i\frac{\partial}{\partial p_i}}\left(\exp\left(i\omega H+\frac{i\omega^2\hbar}{2m}\sum_{i=1}^{D}p_i\frac{\partial V}{\partial x_i}+\frac{i\omega^3\hbar^2}{6m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2\right)\right)$$

(I.5.12)

$$=\ \exp\left(i\omega H+\frac{i\omega^3\hbar^2}{24m}\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2\right)\ .$$

Thus combining (I.5.7) and (I.5.12) we have

$$\boxed{(\text{I.5.13})\quad \rho(\underset{\sim}{p},\underset{\sim}{r})=\frac{-2}{h^D}\cdot\frac{1}{2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{d\omega}{\omega}\,e^{-i\omega(E-H(\underset{\sim}{p},\underset{\sim}{r}))+\frac{i\omega^3\hbar^2}{24m}|\underset{\sim}{\nabla}V|^2}}$$

where $|\underset{\sim}{\nabla}V|^2=\sum_{i=1}^{D}\left(\frac{\partial V}{\partial x_i}\right)^2.$

From (I.5.13) we may immediately compute forms for the space density:

$$(\text{I.5.14})\qquad \rho(\underset{\sim}{r})\ =\ \Omega_D\int_0^\infty\rho(\underset{\sim}{p},\underset{\sim}{r})\,p^{D-1}\,dp$$

and the kinetic energy density:

$$(\text{I.5.15})\qquad t(\underset{\sim}{r})\ =\ \Omega_D\int_0^\infty\rho(\underset{\sim}{p},\underset{\sim}{r})\,\frac{p^2}{2m}\,p^{D-1}\,dp\ .$$

To get $\rho(\underset{\sim}{r})$ and $t(\underset{\sim}{r})$ from (I.5.13) we consider the integral:

$$(\text{I.5.16})\qquad \Omega_D\int_0^\infty e^{\frac{i\omega p^2}{2m}}\,p^{N-1}\,dp\ =\ \frac{\Omega_D}{2}\left(\frac{2m}{\omega}\right)^{N/2}\Gamma\left(\frac{N}{2}\right)e^{\frac{i\pi N}{4}}\ .$$

Combining (I.5.13), (I.5.14) and (I.5.16) we get:

$$\boxed{\begin{aligned}(\text{I.5.17})\quad \rho(\underset{\sim}{r}) = \frac{-\Omega_D}{h^D}(2m)^{D/2}\,\Gamma\left(\frac{D}{2}\right)\frac{e^{\frac{i\pi D}{4}}}{2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{d\omega}{\omega^{\frac{D+2}{2}}}\\ \cdot\; e^{-i\omega(E-V(\underset{\sim}{r}))+\frac{i\omega^3\hbar^2}{24m}|\underset{\sim}{\nabla}V|^2}\end{aligned}}$$

and similarly combining (I.5.13), (I.5.15) and (I.5.16) we get

$$\boxed{\begin{aligned}(\text{I.5.18})\quad t(\underset{\sim}{r}) = \frac{-\Omega_D}{2m\;h^D}\,(2m)^{\frac{D+2}{2}}\,\Gamma\left(\frac{D+2}{2}\right)\frac{e^{\frac{i\pi(D+2)}{4}}}{2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{d\omega}{\omega^{\frac{D+4}{2}}}\\ \cdot\; e^{-i\omega(E-V(\underset{\sim}{r}))+\frac{i\omega^3\hbar^2}{24m}|\underset{\sim}{\nabla}V|^2)}\;.\end{aligned}}$$

Equations (I.5.13), (I.5.17) and (I.5.18) may be written in somewhat neater form.

From (I.5.13):

$$(\text{I.5.19})\quad \frac{\partial\rho(\underset{\sim}{p},\underset{\sim}{r})}{\partial E} = \frac{2}{h^D}\,\frac{1}{2\pi}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon} d\omega\; e^{-i\omega(E-H(\underset{\sim}{p},\underset{\sim}{r}))+\frac{i\omega^3\hbar^2}{24m}|\underset{\sim}{\nabla}V|^2}$$

so that

$$(\text{I.5.20})\quad \frac{\partial\rho(\underset{\sim}{p},\underset{\sim}{r})}{\partial E} = \frac{2}{h^D}\,\frac{2m}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}\,A_i\left(\frac{-2m(E-H(\underset{\sim}{p},\underset{\sim}{r}))}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}\right)$$ [2]

where $A_i(x)$ is the Airy function. Assuming $\rho(\underset{\sim}{p},\underset{\sim}{r})\Big|_{E=-\infty} = 0$ then

$$(\text{I.5.21})\quad \rho(\underset{\sim}{p},\underset{\sim}{r}) = \frac{2}{h^D}\int_{-\infty}^{E} \frac{2m}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}\,A_i\left(\frac{-2m(u-H(\underset{\sim}{p},\underset{\sim}{r}))}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}\right) du$$

or, substituting $t = \dfrac{2m(u-H(\underset{\sim}{p},\underset{\sim}{r}))}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}$, we get:

$$\boxed{(\text{I.5.22})\quad \rho(\underset{\sim}{p},\underset{\sim}{r}) = \frac{2}{h^D}\int_{-\infty}^{\frac{2m(E-H(\underset{\sim}{p},\underset{\sim}{r}))}{|m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}} A_i(-t)\,dt\ .}$$

To get somewhat similar forms for $\rho(\underset{\sim}{r})$ and $t(\underset{\sim}{r})$ we should first recognize that integrating (I.5.14) and (I.5.15) by parts we have:

$$(\text{I.5.23})\qquad \rho(\underset{\sim}{r}) = -\frac{\Omega_D}{D}\int_0^{\infty} p^D\,\frac{\partial\rho(\underset{\sim}{p},\underset{\sim}{r})}{\partial p}\,dp$$

and

$$(\text{I.5.24})\qquad t(\underset{\sim}{r}) = -\frac{\Omega_D}{2m(D+2)}\int_0^{\infty} p^{D+2}\,\frac{\partial\rho(\underset{\sim}{p},\underset{\sim}{r})}{\partial p}\,dp\ .$$

---

[2] Handbook of Math. Functions, edited by Milton Abramowitz and Irene A. Stegun (New York, Dover Publ., Inc, 1965), p. 447 (10.4.32).

From (I.5.13)

$$(\mathrm{I}.5.25)\quad \frac{\partial\rho(\underset{\sim}{p},\underset{\sim}{r})}{\partial p} = \frac{-2}{h^D}\,\frac{p}{m}\,\frac{1}{2\pi}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon} d\omega\; e^{-i\omega(E-H(\underset{\sim}{p},\underset{\sim}{r}))+\frac{i\omega^3\hbar^2}{24m}|\underset{\sim}{\nabla}V|^2}$$

so that

$$(\mathrm{I}.5.26)\quad \frac{\partial\rho(\underset{\sim}{p},\underset{\sim}{r})}{\partial p} = \frac{-2}{h^D}\,\frac{p}{m}\,\frac{2m}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}\,A_i\Big(\frac{-2m(E-V(\underset{\sim}{r})-\frac{p^2}{2m})}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}\Big)\;.$$

Substituting $t = \dfrac{2m[E-V(\underset{\sim}{r})-\frac{p^2}{2m}]}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}$ , we get

$$(\mathrm{I}.5.27)\quad \frac{\partial\rho(\underset{\sim}{p},\underset{\sim}{r})}{\partial p}\,dp = \frac{2}{h^D}\,A_i(-t)\,dt$$

and $\quad p = (m\hbar|\underset{\sim}{\nabla}V|)^{1/3}\Big(\dfrac{2m(E-V(\underset{\sim}{r}))}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}} - t\Big)^{1/2}.$

Thus (I.5.23) becomes

$$\boxed{(\mathrm{I}.5.28)\quad \rho(\underset{\sim}{r}) = \frac{2\,\Omega_D}{h^D\,D}\,(m\hbar|\underset{\sim}{\nabla}V|)^{D/3}\int_{-\infty}^{\alpha}(\alpha-t)^{D/2}\,A_i(-t)\,dt}$$

and (I.5.24) becomes

$$\boxed{(\mathrm{I}.5.29)\quad t(\underset{\sim}{r}) = \frac{2\,\Omega_D}{h^D(2m)(D+2)}\,(m\hbar|\underset{\sim}{\nabla}V|)^{\frac{D+2}{3}}\int_{-\infty}^{\alpha}(\alpha-t)^{\frac{D+2}{2}}\,A_i(-t)\,dt}$$

where

$$\boxed{(\text{I.5.30}) \qquad \alpha = \frac{2m(E-V(\underset{\sim}{r}))}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}} \ .}$$

When D is odd it is possible to integrate (I.5.28) and (I.5.30) explicitly.

From equation (A.3.12), we see that:

$$\boxed{\begin{aligned}(\text{I.5.31}) \quad \rho(\underset{\sim}{r}) &= \frac{(-1)^{\frac{D+1}{2}}\, 4\pi\, \Omega_D}{D\ h^D}\,(2m\hbar|\underset{\sim}{\nabla}V|)^{D/3} \\ &\cdot \frac{d^{D+1}}{du^{D+1}}\, A_i\!\left(\frac{-\alpha}{4^{1/3}}+\frac{u}{2}\right) A_i\!\left(\frac{-\alpha}{4^{1/3}}-\frac{u}{2}\right)\Bigg|_{u=0} , \quad \text{for } D = 1,3,5,\text{etc.},\end{aligned}}$$

and from equation (A.3.11), we see that:

$$\boxed{\begin{aligned}(\text{I.5.32}) \quad t(\underset{\sim}{r}) &= \frac{(-1)^{\frac{D+3}{2}}\, 4\pi\, \Omega_D (2m\hbar|\underset{\sim}{\nabla}V|)^{\frac{D+2}{3}}}{(D+2)\ 2m\ h^D} \\ &\cdot \frac{d^{D+3}}{du^{D+3}}\, A_i\!\left(\frac{-\alpha}{4^{1/3}}+\frac{u}{2}\right) A_i\!\left(\frac{-\alpha}{4^{1/3}}-\frac{u}{2}\right)\Bigg|_{u=0} , \quad \text{for } D = 1,3,5,\ldots \ .\end{aligned}}$$

For the complete asymptotic expansions of $\rho(\underset{\sim}{r})$ and $t(\underset{\sim}{r})$ for arbitrary D the reader should refer to Appendix 4, particularly (A.4.20), (A.4.21), (A.4.22), (A.4.26), (A.4.27) and (A.4.28).

However in the particular case where D = 3, with

$$\alpha \;=\; \frac{2m(E-V(\underset{\sim}{r}))}{(mh|\underset{\sim}{\nabla}V|)^{2/3}} \;>\; 0$$

we find that

$$(I.5.33)\quad \rho(\underset{\sim}{r}) \sim \frac{8\pi}{3h^3}\,[2m(E-V(\underset{\sim}{r}))]^{3/2}\left[1-\frac{1}{8\alpha^3}-\frac{3}{4\alpha^3}\sin\frac{2}{3}\,\alpha^{3/2}\right]$$

$$(I.5.34)\quad t(\underset{\sim}{r}) \sim \frac{4\pi}{5mh^3}\,[2m(E-V(\underset{\sim}{r}))]^{5/2}\left[1+\frac{5}{8\alpha^3}+\frac{15}{8\alpha^3}\cos\frac{2}{3}\,\alpha^{3/2}\right]$$

and, with $\alpha < 0$, we have

$$(I.5.35)\quad \rho(\underset{\sim}{r}) \sim \frac{\pi}{h^3}\,[2m(V(\underset{\sim}{r})-E)]^{3/2}\;\frac{e^{-\frac{2}{3}(-\alpha)^{3/2}}}{(-\alpha)^3}$$

$$(I.5.36)\quad t(\underset{\sim}{r}) \sim \frac{3\pi}{4mh^3}\,[2m(V(\underset{\sim}{r})-E)]^{5/2}\;\frac{e^{-\frac{2}{3}(-\alpha)^{3/2}}}{(-\alpha)^{9/2}}\;.$$

These may of course be regarded as connection formulas.

Of particular interest here is the comparison of (I.5.33) and (I.5.35) with equation (I.4.2). The first two terms of (I.5.33) are the T.F. approximation with Weizsäcker correction as in (I.4.2). However, the third term in (I.5.34) is an oscillatory term with an amplitude 6 times the magnitude of the reduced Weizsäcker term.

It should be noted that this oscillatory term would never have been produced by the method of expansion in powers of $\hbar$. Also the method of expansion in powers of $\hbar$ will never give anything other than zero for the region $V(\underset{\sim}{r}) > E$.

We should also consider the one dimensional case and then compare our result with that of Kohn and Sham [7] and that of Macke and Rennert [6].

For one dimension, equations (A.4.20) and (A.4.21) give us:

$$\text{(I.5.37)} \qquad \rho(r) \sim \frac{4}{h}\,[2m(E-V(r))]^{1/2}\Big[1 - \frac{\cos\frac{2}{3}\beta}{2\beta}\Big] .$$

Now if we continue to make the approximation that $V(r) = a + br$ $(b > 0)$, then

$$\frac{2}{3}\beta = \frac{2}{3}\,\frac{[2m(E-V(r))]^{3/2}}{m\hbar|\underset{\sim}{\nabla}V|} = \frac{2}{\hbar}\int_r^{r_0} [2m(E-V(u)))^{1/2}\,du,$$

where $V(r_0) = E$.

Also:

$$\frac{[2m(E-V(r))]^{1/2}}{mh|\underset{\sim}{\nabla}V|} = \frac{1}{\hbar}\int_r^{r_0} [2m(E-V(u))]^{-1/2}\,du.$$

Now, if we substitute the parameters used by Kohn and Sham,

$$p(E,r) = [2m(E-V(r))]^{1/2}$$

$$\tau(E,r) = \frac{1}{\hbar} \int_{r}^{r_0} [2m(E-V(r))]^{-1/2} \, du$$

$$\theta(E,r) = \frac{1}{\hbar} \int_{r}^{r_0} [2m(E-V(r))]^{1/2} \, du$$

then we get

$$\text{(I.5.38)} \qquad \rho(r) \sim \frac{2}{\pi\hbar} \left[p(E,r) - \frac{\cos 2\theta(E,r)}{2p(E,r)\tau(E,r)}\right]$$

which aside from our spin factor of 2 is precisely the result of Kohn and Sham.[3]

Note! Although equation (I.5.37) agrees with the result of Kohn and Sham, it does not agree with the result of Macke and Rennert. It appears that P. Rennert (it was his dissertation) made some error in computing his asymptotic expansion. In both the Macke-Rennert paper and Kohn-Sham paper graphical comparisons were made of exact and approximate solutions for harmonic oscillator and Coulomb potentials. These graphical comparisons are a little disappointing in the Macke-Rennert paper whereas they were excellent in the Kohn-Sham paper. The only significant error on the Kohn-Sham graphs appears for the Coulomb potential when r is near zero. And perhaps this region should be attacked differently.

---

[3] W. Kohn and L. J. Sham, Phys. Rev. 137 A 1701 (1965) equations (3.14), (3.15) and (3.16)

## Section 6. Relation to W.K.B. Method.

First of course we have made the approximation that $\partial^2 V/\partial x_i \partial x_j = 0$, which is done in the transition region for the W.K.B. method.

Now if $V = \underset{\sim}{a} \cdot \underset{\sim}{r} + b$ where $\underset{\sim}{a}$ is a constant vector and b is a constant scalar and $E > V(\underset{\sim}{r})$ then

$$(I.6.1) \quad \underset{\sim}{\nabla} \frac{2}{3} \alpha^{3/2} = \underset{\sim}{\nabla} \frac{2}{3} \frac{[2m(E-V(\underset{\sim}{r}))]^{3/2}}{mh|\underset{\sim}{\nabla} V|} = \frac{2}{\hbar} [2m(E-V(\underset{\sim}{r}))]^{1/2} \frac{(-\underset{\sim}{a})}{|\underset{\sim}{a}|}$$

Thus

$$(I.6.2) \quad \frac{2}{3} \alpha^{3/2} = \frac{2}{\hbar} \int_{\underset{\sim}{r}_0}^{\underset{\sim}{r}} [2m(E-V(\underset{\sim}{u}))]^{1/2} \frac{(-\underset{\sim}{a})}{|\underset{\sim}{a}|} \cdot d\underset{\sim}{u} \quad ,$$

where $\underset{\sim}{r}_0$ is a value such that $V(\underset{\sim}{r}_0) = E$.

For an attractive potential in one dimension, $+\underset{\sim}{a} = |\underset{\sim}{a}|$ and

$$(I.6.3) \quad \frac{2}{3} \alpha^{3/2} = \frac{2}{\hbar} \int_{r}^{r_0} [2m(E-V(u))]^{1/2} du \ .$$

For E < V, and proceeding similarly, we get:

$$(I.6.4) \quad \frac{2}{3} (-\alpha)^{3/2} = \frac{2}{\hbar} \int_{\underset{\sim}{r}_0}^{\underset{\sim}{r}} [2m(V(\underset{\sim}{u})-E)]^{1/2} \frac{\underset{\sim}{a}}{|\underset{\sim}{a}|} \cdot d\underset{\sim}{u}$$

And here again for a one dimensional attractive potential we have the form

$$(\mathrm{I.6.5}) \quad \frac{2}{3}(-\alpha)^{3/2} = \frac{2}{\hbar}\int_{\underset{\sim}{r}_0}^{\underset{\sim}{r}} [2m(V(\underset{\sim}{u})-E)]^{1/2}\, du \ .$$

Of course when $\underset{\sim}{\nabla} V$ is not a constant vector (I.6.2) and (I.6.4) are no longer identities.

If for example we assume that the potential experienced by electrons of an atom at long range is $-e^2/r$, then:

$$(\mathrm{I.6.6}) \qquad \frac{2}{3}(-\alpha)^{3/2} \sim \frac{2}{3}\,\frac{[2m(-E)]^{3/2}\, r^2}{m\,\hbar\, e^2}$$

whereas

$$(\mathrm{I.6.7}) \qquad \frac{2}{\hbar}\int_{r_0}^{r} [2m(V(\underset{\sim}{u})-E)]^{1/2}\, du \sim \frac{2[2m(-E)]^{1/2}\, r}{\hbar} \ .$$

Looking at (I.5.35) it appears that for long range it would be more appropriate to use approximation (I.6.7) rather than (I.6.6).

## Section 7. Region Near Nucleus of an Atom.

It appears that our approximation should be good in the transition region where $E - V(r)$ is dominated by its linear part. Our approximation should also be good in the oscillatory and exponentially decreasing regions particularly if we replace $\frac{2}{3}\,(\pm\,\alpha)^{3/2}$ by the appropriate W.K.B. integral.

However a glance at equation (I.5.28) shows that we have a disaster for $r \approx 0$. If $V = -\,Ze^2/r$ then $|\underset{\sim}{\nabla} V| = Ze^2/r^2$ so $\rho(\underset{\sim}{r}) = O(1/r^2)$. This singularity is such that the integral for the total potential energy:

$$- 4\pi \int_0^\infty \frac{Ze^2}{r}\, \rho(r)\, r^2\, dr \qquad \text{would not exist.}$$

One way to avoid this difficulty is to rewrite (I.5.28) for $D = 3$ in the form

$$\text{(I.7.1)} \qquad \rho(\underset{\sim}{r}) = \frac{8\pi}{3h^3}\, [2m(E-V(\underset{\sim}{r}))]^{3/2} \int_{-\infty}^{\alpha} (1 - \frac{t}{\alpha})^{3/2}\, A_i(-t)\, dt$$

and replace $\frac{2}{3}\,\alpha^{3/2}$ which equals zero at $r = 0$ by $\frac{2}{\hbar} \int_r^{Ze^2/(-E)} [2m(E + \frac{Ze^2}{r})]^{1/2}\, dr$, which is not zero at $r = 0$.

However it should be noted that the justifications for a W.K.B. approximation break down in this region. And Kirzhnits for one states that a large amount of the error in T.F. total energy computations comes from just this region.

So now let us consider some other way of handling the situation.

$$(\mathrm{I}.7.2) \qquad \rho(\underset{\sim}{r}) = 2 \sum_{k=1}^{A} \psi_k(\underset{\sim}{r})\, \psi_k^*(\underset{\sim}{r})$$

$$(\mathrm{I}.7.3) \qquad \psi_k(\underset{\sim}{r}) = e^{-Zr/na_0} \cdot O(r^{\ell})$$ [4]

where $\ell$ is the azimuthal number, $n$ the total quantum number and $a_0$ = the first hydrogen Bohr orbit = $\hbar^2/me^2$. Thus we see that near the nucleus $\rho(\underset{\sim}{r})$ is dominated by the s states.

For an s state:

$$(\mathrm{I}.7.4) \quad \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial r^2} \psi_k(r) - \frac{\hbar^2}{mr} \frac{\partial \psi_k(r)}{\partial r} - \frac{Ze^2}{r} \psi_k(r) = E_k \psi_k(r).$$

Multiplying (I.7.4) by r and then letting r approach zero, the important terms of (I.7.4) become:

$$(\mathrm{I}.7.5) \qquad -\frac{\hbar^2}{m} \frac{\partial \psi_k(r)}{\partial r} - Ze^2\, \psi_k(r) = 0 .$$

Multiplying (I.7.5) by $\psi_k^*(r)$ we get:

$$(\mathrm{I}.7.6) \qquad -\frac{\hbar^2}{m} \psi_k^*(r) \frac{d}{dr} \psi_k(r) - Ze^2\, \psi_k^*(r)\, \psi_k(r) = 0.$$

Adding (I.7.6) to its complex conjugate we have:

---

[4] Leonard I. Schiff, *Quantum Mechanics* (New York, McGraw-Hill Book Co., Inc., 1955) p. 85.

$$(\text{I.7.7}) \qquad -\frac{\hbar^2}{m}\frac{d}{dr}\left(\psi_k^*(r)\psi_k(r)\right) - 2\,Ze^2\,\psi_k^*(r)\,\psi_k(r) = 0.$$

Summing over all s states we have

$$(\text{I.7.8}) \qquad -\frac{\hbar^2}{m}\frac{\partial}{\partial r}\sum_{\text{s states}}\psi_k^*(r)\psi_k(r) - 2\,Ze^2\sum_{\text{s states}}\psi_k^*(r)\psi_k(r) = 0\,,$$

or

$$(\text{I.7.9}) \qquad \frac{\frac{\partial}{\partial r}\sum_{\text{s states}}\psi_k^*(r)\,\psi_k(r)}{\sum_{\text{s states}}\psi_k^*(r)\,\psi_k(r)} = -\frac{2Z}{a_0} \quad \text{for r near 0.}$$

Now referring to (I.7.2) and (I.7.3) it is clear that

$$(\text{I.7.10}) \qquad \frac{d}{dr}\rho(r) = \frac{d}{dr}\sum_{\text{s states}}\psi_k^*(r)\,\psi_k(r) \quad \text{for r near 0;}$$

and

$$\rho(r) = \sum_{\text{s states}}\psi_k^*(r)\,\psi_k(r) \qquad \text{for r near 0.}$$

Thus the appropriate condition to use on $\rho(r)$ for r near zero is

$$\boxed{(\text{I.7.11}) \qquad \left.\frac{\partial\rho(r)}{\partial r}\middle/\rho(r)\right|_{r=0} = -\frac{2Z}{a_0}}$$

where $a_0 = \hbar^2/me^2$.

Now let us turn to the kinetic energy density.

$$t(\underset{\sim}{r}) = \iint \rho(\underset{\sim}{p},\underset{\sim}{r}) \frac{p^2}{2m} d\underset{\sim}{p} \; . \tag{I.7.12}$$

On the other hand taking the Fourier transform of equation (A.1.12) we have

$$\iint \rho(\underset{\sim}{p},\underset{\sim}{r})\, e^{i\underset{\sim}{\tau}\cdot\underset{\sim}{p}}\, d\underset{\sim}{p} = 2\sum_{k} \psi_k(\underset{\sim}{r}+\frac{\hbar}{2}\,\underset{\sim}{\tau})\psi_k^*(\underset{\sim}{r}-\frac{\hbar}{2}\,\underset{\sim}{\tau}) . \tag{I.7.13}$$

From (I.7.12) for D = 3

$$t(\underset{\sim}{r}) = -\frac{1}{2m}\sum_{j=1}^{3}\frac{\partial^2}{\partial\tau_j^2}\iint \rho(\underset{\sim}{p},\underset{\sim}{r})\, e^{i\underset{\sim}{\tau}\cdot\underset{\sim}{p}}\, d\underset{\sim}{p}\,\Big|_{\underset{\sim}{\tau}=\underset{\sim}{0}} \; . \tag{I.7.14}$$

Thus from (I.7.13) and (I.7.14)

$$t(\underset{\sim}{r}) = -2\left(\frac{1}{2m}\right)\frac{\hbar^2}{4}\sum_{k}\left[(\nabla_k^2\psi_k(\underset{\sim}{r}))\psi_k^*(\underset{\sim}{r}) - 2\underset{\sim}{\nabla}\psi_k(\underset{\sim}{r})\cdot\underset{\sim}{\nabla}\psi_k^*(\underset{\sim}{r}) + \psi_k(\underset{\sim}{r})\nabla^2\psi_k^*(\underset{\sim}{r})\right] \tag{I.7.15}$$

but since

$$-\frac{\hbar^2}{2m}\nabla^2\psi_k = (E_k - V(\underset{\sim}{r}))\psi_k ,$$

we may write

$$t(\underset{\sim}{r}) = \sum_{k}\left(E_k\psi_k(\underset{\sim}{r})\psi_k^*(\underset{\sim}{r}) - V(\underset{\sim}{r})\psi_k(\underset{\sim}{r})\psi_k^*(\underset{\sim}{r}) + \frac{h^2}{2m}\underset{\sim}{\nabla}\psi_k\cdot\underset{\sim}{\nabla}\psi_k^*\right) . \tag{I.7.16}$$

Substituting $V(\underset{\sim}{r}) = -Ze^2/r$, multiplying (I.7.16) by r and then letting r approach zero we have

$$\boxed{(\text{I.7.17}) \qquad \left.\frac{r\,t(\underset{\sim}{r})}{\rho(\underset{\sim}{r})}\right|_{r=0} = \frac{Ze^2}{2}\ .}$$

Section 8. Bohr Sommerfeld Rule for Hydrogen Atom.

If we use $V(\underset{\sim}{r}) = -Ze^2/r$ then $\rho(\underset{\sim}{r}) = 2\sum_{k=1}^{N} \psi_k(\underset{\sim}{r})\psi_k^*(\underset{\sim}{r})$ a sum over the first N solutions of the hydrogen atom.

Also E, the T.F. cut-off energy or chemical potential if you wish, has the property that

$$E_N < E < E_{N+1}\ .$$

Now from (I.5.33) and (I.5.34)

$$(\text{I.8.1}) \qquad \frac{r\,t(\underset{\sim}{r})}{\rho(\underset{\sim}{r})} \approx \frac{3}{5}\,(Ze^2 + Er)\,\frac{\left[1 + \frac{5}{8\alpha^3} + \frac{15}{8\alpha^3}\cos\frac{2}{3}\alpha^{3/2}\right]}{\left[1 - \frac{1}{8\alpha^3} - \frac{3}{4\alpha^3}\sin\frac{2}{3}\alpha^{3/2}\right]}$$

but

$$(\text{I.7.17}) \qquad \left.\frac{r\,t(\underset{\sim}{r})}{\rho(\underset{\sim}{r})}\right|_{r=0} = \frac{1}{2}\,Ze^2.$$

Equations (I.7.17) and (I.8.1) seem to suggest that at $r = 0$ the W.K.B. integral corresponding to $\frac{2}{3}\alpha^{3/2}$ should be an angle in the second quadrant. Thus

$$(\mathrm{I.8.2}) \qquad \frac{2}{\hbar} \int_{0}^{Ze^2/(-E)} \left[2m\left((+E) + \frac{Ze^2}{r}\right)\right]^{1/2} dr = (2n + \Delta)\pi$$

where n is an integer.

Carrying out the integration we get:

$$(\mathrm{I.8.3}) \qquad E = -\frac{Z^2e^2}{2a_0\left(n + \frac{\Delta}{2}\right)^2} \qquad \text{where } \frac{1}{2} < \Delta < 1.$$

Of course to get E more accurately we should adjust E so it satisfies the equation:

$$\int \rho(\underset{\sim}{r})\, d\underset{\sim}{r} = N \qquad \text{where N is the number of electrons.}$$

# Part II

## Section 1. Exact Wigner-Moyal Density for Non-Interacting Harmonic Oscillator.

When discussing approximation schemes it is nice to have some exact solutions for points of reference. First they provide a test of sorts for the accuracy of any given approximation scheme. And secondly they may provide starting points for other approximation schemes. Thus in Sections 1 and 2 of Part II we will discuss solutions to a system of N non-interacting bodies in a D dimensional, spherically symmetric, harmonic oscillator potential.

In Sections 3 to 5 of Part II we will discuss a system of interacting harmonic oscillators.

Consider first the one dimensional harmonic oscillator

$$-\frac{h^2}{2m}\frac{d^2u}{dx^2} + \frac{1}{2}\,k\,x^2u \;=\; Eu\;. \tag{II.1.1}$$

This equation has normalized solutions

$$u_n(x) \;=\; N_n\,H_n\,(\alpha x)\,e^{-\frac{1}{2}\alpha^2x^2}\;,\quad ^{5/} \tag{II.1.2}$$

---

5/ Schiff, Quantum Mechanics, p. 64.

with corresponding eigenvalue $E_n = (n+\frac{1}{2})\hbar\omega c$, $\omega c = \sqrt{k/m}$, where $N_n = (\alpha/\pi^{1/2} 2^n n!)^{1/2}$ and $\alpha^4 = mk/h^2$.

Now since the equation:

$$(\text{II.1.3}) \qquad -\frac{\hbar^2}{2m} \sum_{i=1}^{D} \frac{\partial^2}{\partial x_i^2} u + \frac{1}{2} k|\underset{\sim}{x}|^2 u = Eu$$

is separable, it is clear that (II.1.3) has normalized solutions of the form:

$$(\text{II.1.4}) \quad u_{m_1,m_2,\ldots,m_D}(\underset{\sim}{x}) = \left[\prod_{j=1}^{D} N_{m_j} H_{m_j}(\alpha x_j)\right] e^{-\frac{1}{2}\alpha^2|\underset{\sim}{x}|^2}$$

with eigenvalue

$$E_m = \left(\sum_{j=1}^{D} m_j + \frac{D}{2}\right) \hbar\omega_c .$$

Now if we introduce the notation that

$$(\text{II.1.5}) \quad H_n^1(\alpha x,\alpha y) = \frac{H_n(\alpha x)H_n(\alpha y)}{2^n\ n!} = \frac{\pi^{1/2}}{\alpha}(N_n^2 H_n(\alpha x)H_n(\alpha y))$$

and

$$(\text{II.1.6}) \quad H_m^D(\alpha\underset{\sim}{x},\alpha\underset{\sim}{y}) = \sum_{m_1+m_2+\cdots m_D=m} H_{m_1}^1(\alpha x_1,\alpha y_1)H_{m_2}^1(\alpha x_2,\alpha y_2) \ldots H_{m_D}^1(\alpha x_D,\alpha y_D).$$

Then we may write the Dirac density for the complete set of states with energy eigenvalue $E_n = (n + \frac{D}{2})\hbar\omega_c$ as

$$(\text{II.1.7}) \qquad \rho_n(\underset{\sim}{x},\underset{\sim}{y}) = (\frac{\alpha^2}{\pi})^{D/2} H_n^D(\alpha\underset{\sim}{x},\alpha\underset{\sim}{y})\, e^{-\frac{\alpha^2}{2}(|\underset{\sim}{x}|^2+|\underset{\sim}{y}|^2)} .$$

And then we will designate the Dirac density corresponding to the complete set of states in the first N "shells" as

$$(\text{II.1.8}) \qquad \rho^N(\underset{\sim}{x},\underset{\sim}{y}) = \sum_{n=0}^{N-1} \rho_n(\underset{\sim}{x},\underset{\sim}{y}) =$$

$$(\frac{\alpha^2}{\pi})^{D/2} \sum_{n=0}^{N-1} H_n^D(\alpha\underset{\sim}{x},\alpha\underset{\sim}{y})\, e^{-\frac{\alpha^2}{2}(|\underset{\sim}{x}|^2+|\underset{\sim}{y}|^2)}$$

where each "shell" corresponds to the complete set of states corresponding to one energy eigenvalue.

Now

$$(\text{II.1.9}) \qquad \sum_{n=0}^{\infty} H_n^1(x,y)z^n = (1-z^2)^{-1/2} \exp\left[\frac{2xyz-(x^2+y^2)z^2}{1-z^2}\right] .$$ [6/]

Thus

$$(\text{II.1.10}) \qquad \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \cdots \sum_{m_D=0}^{\infty} z^{m_1+m_2+\cdots m_D} \cdot$$

$$H_{m_1}^1(x_1,y_1)\, H_{m_2}^1(x_2,y_2) \cdots H_{m_D}^1(x_D,y_D) =$$

---

[6/] Bateman Manuscript Project, Higher Transcendental Functions, Vol. II (New York, McGraw-Hill Book Co., Inc. 1953), p. 194, eq. (22).

$$= (1-z^2)^{-D/2} \exp\left[\frac{2\underset{\sim}{x}\cdot\underset{\sim}{y}z - (|\underset{\sim}{x}|^2+|\underset{\sim}{y}|^2)z^2}{1 - z^2}\right]$$

or

$$\text{(II.1.11)} \quad \sum_{m=0}^{\infty} z^m H_m^D(\underset{\sim}{x},\underset{\sim}{y}) = (1-z^2)^{-D/2} \exp\left|\frac{2\underset{\sim}{x}\cdot\underset{\sim}{y}z-(\underset{\sim}{x}^2+|\underset{\sim}{y}|^2)z^2}{1-z^2}\right| .$$

Let

$$\underset{\sim}{x} = \underset{\sim}{R} + \underset{\sim}{r}\,, \quad \underset{\sim}{x}\cdot\underset{\sim}{y} = R^2 - r^2 \quad \text{where } R = |\underset{\sim}{R}|;$$

$$\underset{\sim}{y} = \underset{\sim}{R} - \underset{\sim}{r}\,, \quad |\underset{\sim}{x}|^2+|\underset{\sim}{y}|^2=2R^2+2r^2 \quad \text{and } r = |\underset{\sim}{r}|;$$

then:

$$\text{(II.1.13)} \quad \sum_{m=0}^{\infty} z^m H_m^D(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = (1-z^2)^{-D/2} \exp\left[\frac{2R^2z}{1+z} - \frac{2r^2z}{1-z}\right].$$

Multiplying both sides by $(1-z)^{-1}$ we get:

$$\text{(II.1.14)} \quad \sum_{k=1}^{\infty} z^{k-1} \sum_{m=0}^{k-1} H_m^D(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})$$

$$= (1-z)^{-1}(1-z^2)^{-D/2} \exp\left|\frac{2R^2z}{1+z} - \frac{2r^2z}{1-z}\right| .$$

Combining (II.1.7) with (II.1.13) we get

$$\text{(II.1.15)} \quad \sum_{m=0}^{\infty} z^m \rho_m(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{\alpha^2}{\pi}\right)^{D/2} (1-z^2)^{-D/2} \cdot$$

$$\exp\left[\frac{-\alpha^2R^2(1-z)}{1+z} - \frac{\alpha^2(1+z)}{1-z}\right] ,$$

where $\rho_m(\underset{\sim}{x},\underset{\sim}{y})$ is the Dirac density of the (m+1)-th shell. Combining (II.1.8) with (II.1.14)

$$\text{(II.1.16)} \quad \sum_{N=1}^{\infty} z^{N-1}\rho^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{\alpha^2}{\pi}\right)^{D/2}(1-z)^{-1}(1-z^2)^{-D/2} \cdot \\ \cdot \exp\left[\frac{-\alpha^2R^2(1-z)}{1+z} - \frac{\alpha^2r^2(1+z)}{1-z}\right],$$

where $\rho^N(\underset{\sim}{x},\underset{\sim}{y})$ is the Dirac density for the first N "shells."

From (A.1.12)

$$\text{(II.1.17)} \quad \rho(\underset{\sim}{p},\underset{\sim}{R}) = \frac{2^D}{h^D}\iint d\underset{\sim}{r}\;\rho(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})\; e^{-\frac{2i\underset{\sim}{r}\cdot\underset{\sim}{p}}{\hbar}} .$$

It can be shown that

$$\text{(II.1.18)} \quad \frac{2^D}{h^D}\iint d\underset{\sim}{r}\; e^{-\frac{2i\underset{\sim}{r}\cdot\underset{\sim}{p}}{\hbar}}\; e^{-\alpha^2r^2\left(\frac{1+z}{1-z}\right)} \\ = \frac{2^D}{h^D}\,\frac{\pi^{D/2}}{\alpha^D}\left(\frac{1-z}{1+z}\right)^{D/2} e^{-\frac{p^2}{\hbar^2\alpha^2}\left(\frac{1-z}{1+z}\right)} .$$

From (II.1.15), (II.1.17) and (II.1.18) we get

$$\text{(II.1.19)} \quad \sum_{m=0}^{\infty} z^m\rho_m(\underset{\sim}{p},\underset{\sim}{R}) = \frac{2^D}{h^D}(1+z)^{-D}\exp\left[-\left(\alpha^2R^2+\frac{p^2}{\hbar^2\alpha^2}\right)\left(\frac{1-z}{1+z}\right)\right].$$

Similarly from (II.1.16), (II.1.17) and (II.1.18) we get:

$$\text{(II.1.20)} \quad \sum_{k=1}^{\infty} z^{N-1}\rho^N(\underset{\sim}{p},\underset{\sim}{R}) = \frac{2^D}{h^D}(1-z)^{-1}(1+z)^{-D}\cdot \\ \cdot \exp\left[-\left(\alpha^2R^2+\frac{p^2}{\hbar^2\alpha^2}\right)\left(\frac{1-z}{1+z}\right)\right] .$$

Now $\alpha^4 = mk/\hbar^2$, so that:

$$(\text{II.1.21})\quad \frac{\rho^2}{\hbar^2\alpha^2} + \alpha^2 R^2 = \frac{2}{\hbar\omega_c}\left(\frac{p^2}{2m} + \frac{k}{2}R^2\right) = \frac{2}{\hbar\omega_c} H(\rho,\underset{\sim}{R})$$

where $\omega_c = \sqrt{k/m}$.

Thus from (II.1.19) and (II.1.21) we have

$$(\text{II.1.22})\quad \sum_{m=0}^{\infty} z^m \rho_m(\underset{\sim}{p},\underset{\sim}{R}) = \frac{2^D}{h^D}(1+z)^{-D}\exp\left[\frac{4}{\hbar\omega_c} H(\underset{\sim}{p},\underset{\sim}{r})\left(\frac{z}{z+1}\right)\right]\cdot$$

$$\cdot \exp\left(\frac{-2H}{\hbar\omega_c}\right),$$

but

$$(\text{II.1.23})\quad (1+z)^{-D}\exp\left[\frac{4}{h\omega_c} H(\underset{\sim}{p},\underset{\sim}{R})\left(\frac{z}{z+1}\right)\right]$$

$$= \sum_{m=0}^{\infty} (-z)^m L_m^{D-1}\left(\frac{4}{\hbar\omega_c} H(\underset{\sim}{p},\underset{\sim}{r})\right),$$ [7]

where $L_m^{D-1}$ is an associated Laguerre polynomial.

Thus

$$\boxed{(\text{II.1.24})\quad \rho_m(\underset{\sim}{p},\underset{\sim}{R}) = \frac{2^D}{h^D}(-1)^m \exp\left(\frac{-2H(\underset{\sim}{p},\underset{\sim}{R})}{\hbar\omega_c}\right) L_m^{D-1}\left(\frac{4}{\hbar\omega_c} H(\underset{\sim}{p},\underset{\sim}{R})\right),}$$

where $\rho_m(\underset{\sim}{p},\underset{\sim}{R})$ is the Wigner-Moyal density for the (m+1)-th "shell."

---

[7] Bateman Project, *Higher Transcendental Functions*, Vol. II, ..., p. 189, eq. (17).

From (II.1.20) and (II.1.21) it is clear that

$$\text{(II.1.25)}\quad \frac{d}{dH}\sum_{N=1}^{\infty} z^{N-1}\rho^{N}(\underset{\sim}{p},\underset{\sim}{R}) = -\left(\frac{2}{\hbar\omega_c}\right)\frac{2^D}{h^D}(1+z)^{-(D+1)} \cdot\exp\left[\frac{4}{\hbar\omega_c}H(\underset{\sim}{p},\underset{\sim}{R})\left(\frac{z}{z+1}\right)\right]\exp\left(\frac{-2H}{\hbar\omega_c}\right)$$

but from (II.1.23)

$$\text{(II.1.26)}\quad \frac{d}{dH}\rho^{N}(\underset{\sim}{p},\underset{\sim}{R}) = \left(\frac{2}{\hbar\omega_c}\right)\frac{2^D}{h^D}(-1)^{N}\exp\left(\frac{-2H(\underset{\sim}{p},\underset{\sim}{R})}{\hbar\omega_c}\right)L^{D}_{N-1}\left(\frac{4}{\hbar\omega_c}H(\underset{\sim}{p},\underset{\sim}{r})\right).$$

Let $u = \frac{4}{\hbar\omega_c}H$, $dH = \frac{\hbar\omega_c}{4}du$. Then

$$\boxed{\text{(II.1.27)}\qquad \rho^{N}(\underset{\sim}{p},\underset{\sim}{R}) = \frac{(-1)^{N+1}}{2}\frac{2^D}{h^D}\int_{\frac{4}{\hbar\omega_c}H}^{\infty} e^{-u/2}\,L^{D}_{N-1}(u)\,du\ .}$$

To get $\rho(\underset{\sim}{R})$ and $t(\underset{\sim}{R})$ we note that

$$\text{(II.1.28)}\qquad \rho(\underset{\sim}{R}) = \Omega_D\int_0^{\infty} p^{D-1}\rho^{N}(\underset{\sim}{p},\underset{\sim}{R})\,dp$$

$$= -\frac{\Omega_D}{D}\int_0^{\infty} p^{D}\frac{\partial\rho^{N}(\underset{\sim}{p},\underset{\sim}{R})}{\partial p}\,dp\ ;$$

and similarly

$$(\mathrm{II.1.29}) \quad t(\underset{\sim}{R}) = \Omega_D \int_0^\infty p^{D-1} \left(\frac{p^2}{2m}\right) \rho^N(\underset{\sim}{p},\underset{\sim}{R})\, dp$$

$$= - \frac{\Omega_D}{2m(D+2)} \int_0^\infty p^{D+2} \frac{\partial \rho^N(\underset{\sim}{p},\underset{\sim}{R})}{\partial p}\, dp$$

but from (II.1.27)

$$(\mathrm{II.1.30}) \quad \frac{\partial \rho^N(\underset{\sim}{p},\underset{\sim}{R})}{\partial p} = (-1)^N \frac{2^D}{h^D} \frac{2p}{(m\hbar\omega_c)} e^{-\frac{2}{\hbar\omega_c} H(\underset{\sim}{p},\underset{\sim}{R})} \cdot$$

$$\cdot\, L^D_{N-1}\left(\frac{4}{\hbar\omega_c} H(\underset{\sim}{p},\underset{\sim}{R})\right) .$$

The corresponding approximation in Part I was

$$(\mathrm{I.5.26}) \quad \frac{\partial \rho(\underset{\sim}{p},\underset{\sim}{R})}{\partial p} = \frac{-2}{h^D} \frac{2p}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}} A_i\left(\frac{2m(H(\underset{\sim}{p},\underset{\sim}{R})-E)}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}\right).$$

To compare (II.1.30) and (I.5.26), we proceed as follows:

For N-th shell, $E_N = (N-1+ D/2)\hbar\omega_c$, so let

$$(\mathrm{II.1.31}) \quad E = (N - 1 + \frac{D}{2} + \frac{1}{2})\hbar\omega_c = \frac{N_D}{4} \hbar\omega_c$$

$$(\mathrm{II.1.32}) \quad 2mV = 2m(V-E) + \frac{N_D}{2} (m\hbar\omega_c).$$

But since $V = \frac{1}{2} k|\underset{\sim}{x}|^2$ and $\omega_c = \sqrt{k/m}$ ,

$$(\mathrm{II.1.33}) \quad 2mV = \frac{|\underset{\sim}{\nabla}V|^2 m}{k} = \frac{(m\hbar\, |\underset{\sim}{\nabla}V|)^2}{(m\hbar\, \omega_c)^2}$$

Equating (II.1.32) and (II.1.33) we get:

$$\text{(II.1.34)} \quad \frac{N_D}{2}(m\hbar\omega_c)^3 - (2m(E-V))(m\hbar\omega_c)^2 - [m\hbar|\underset{\sim}{\nabla}V|]^2 = 0.$$

This may be regarded as a cubic equation in $(m\hbar\omega_c)$:

The real solution to (II.1.34) is

$$\text{(II.1.35)} \qquad m\hbar\omega_c = \frac{2^{1/3}[m\hbar\,|\underset{\sim}{\nabla}V|]^{2/3}}{N_D^{1/3}} f(\alpha) ,$$

where

$$\text{(II.1.36)} \qquad f(\alpha) = \frac{1}{2^{1/3}}\left[\sqrt[3]{1+\frac{8\alpha^3}{27N_D^2}+\sqrt{1+\frac{16\alpha^3}{27N_D^2}}} + \sqrt[3]{1+\frac{8\alpha^3}{27N_D^2}-\sqrt{1+\frac{16\alpha^3}{27N_D^2}}}\right]$$

and

$$\text{(II.1.37)} \qquad \alpha = \frac{2m(E-V(\underset{\sim}{r}))}{(m\hbar\,|\underset{\sim}{\nabla}V|)^{2/3}}$$

Now $H = H-E + N_D\hbar\omega_c/4$, so that

$$\text{(II.1.38)} \qquad \frac{4H}{\hbar\omega_c} = N_D + \frac{4m(H-E)}{m\hbar\omega_c}$$

and from (II.1.35) we get:

$$(\mathrm{II}.1.39)\qquad \frac{4H}{\hbar\omega_c} = N_D + \frac{2m(H-E)}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}\, f(\alpha)}\,(4\,N_D)^{1/3}$$

but for large values of $N_D = 4(N-1) + 2D + 2$ and small values of s:

$$(\mathrm{II}.1.40)\qquad e^{-u/2}\, L^{D}_{N-1}(u)\Big|_{N_D+(4N_D)^{1/3}s} \sim \frac{(-1)^{N-1}\,2^{-D}\,2^{1/3}}{N_D^{1/3}}\, A_i(s),$$ [8]

and

$$(\mathrm{II}.1.41)\qquad f(\alpha) \sim 1 \quad \text{for large } N_D.$$

Thus from (II.1.30) and (II.1.35)

$$(\mathrm{II}.1.42)\qquad \frac{\partial\rho^{N}(\underset{\sim}{p},\underset{\sim}{R})}{\partial p} \sim \frac{-1}{2^D}\,\frac{2p}{[m\hbar|\underset{\sim}{\nabla}V|]^{2/3}}\, A_i\!\left(\frac{2m(H-E)}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}}\right)$$

which aside from a factor of 2 is exactly the approximation (I.5.26). The factor of 2 is caused by the fact that we included a spin factor of 2 in all equations of Part I but not Part II.

---

[8] Bateman Project, Higher Transcendental Functions, II, p. 200, equations (10-(13). It should be noted that the Airy function in Bateman, $A(t) = \pi/3^{1/3}\, A_i(-t/3^{1/3})$ where $A_i(t)$ is the Airy function of the Handbook of Math. Functions used in this paper.

To justify the substitution of approximation (II.1.42) in integrals (II.1.28) and (II.1.29) to compute $\rho(\underset{\sim}{r})$ and $t(\underset{\sim}{r})$ respectively, we should note that

$$p^{D-1}\Big|\frac{-2p}{2^D[m\hbar|\underset{\sim}{\nabla}V|]^{2/3}}\;A_i\Big(\frac{2m(H-E)}{[m\hbar|\underset{\sim}{\nabla}V|]^{2/3}}\Big)$$

as an integrand makes the larges contribution to integrals (II.1.28) and (II.1.29) in the part of its domain where it is most accurate as an approximation of $p^{D-1}\dfrac{\partial\rho^N(\underset{\sim}{p},\underset{\sim}{R})}{\partial p}$ namely for $H(\underset{\sim}{p},\underset{\sim}{R})$ near E.

To summarize, the exact integrals are

$$\text{(II.1.43)}\qquad \rho^N(\underset{\sim}{p},\underset{\sim}{R}) = \frac{1}{h^D}\int_{-\infty}^{\frac{2m(E-H)}{(m\hbar|\underset{\sim}{\nabla}V|)^{2/3}f(\alpha)}} (-1)^{N+1}2^D\left(\frac{N_D}{2}\right)^{1/3}\cdot\, e^{-u/2}\,L^D_{N-1}(u)\Big|_{u=N_D-(4N_D)^{1/3}t}\,dt$$

$$\text{(II.1.44)}\qquad \rho(\underset{\sim}{R}) = \frac{\Omega_D}{h^D D}[m\hbar|\underset{\sim}{\nabla}V|]^{D/3}\int_{-\infty}^{\frac{\alpha}{f(\alpha)}}\left[\frac{\alpha}{f(\alpha)}-t\right]^{D/2}[f(\alpha)]^{D/2}\cdot\,(-1)^{N+1}2^D\left(\frac{N_D}{3}\right)^{1/3}e^{-u/2}L^D_{N-1}(u)\Big|_{u=N_D-(4N_D)^{1/3}t}\,dt$$

$$(\text{II.1.45}) \quad t(\underset{\sim}{R}) = \frac{\Omega_D [mh|\underset{\sim}{\nabla} V|]^{\frac{D+2}{3}}}{2m\ h^D (D+2)} \int_{-\infty}^{\frac{\alpha}{f(\alpha)}} [\frac{\alpha}{f(\alpha)} - t]^{\frac{D+2}{2}} [f(\alpha)]^{\frac{D+2}{2}} \cdot$$

$$\cdot \quad (-1)^{N+1} 2^D (\frac{N_D}{3})^{1/3} e^{-u/2} L^D_{N-1}(u) \Big|_{u=N_D-(4N_D)^{1/3}t} \quad dt$$

where

$$f(\alpha) = \frac{1}{2^{1/3}} \left[ \sqrt[3]{1 + \frac{8\alpha^3}{27N_D^2} + \sqrt{1 + \frac{16\alpha^3}{27N_D^2}}} + \sqrt[3]{1 + \frac{8\alpha^3}{27N_D^2} - \sqrt{1 + \frac{16\alpha^3}{27N_D^2}}} \right]$$

and as in Part I $\alpha = \dfrac{2m(E-V(\underset{\sim}{r}))}{(m\hbar\ |\underset{\sim}{\nabla} V|)^{2/3}}$

but for large values of $N_D = 4N + 2D - 2$,

$f(\alpha) \sim 1$

$$(-1)^{N+1} 2^D (\frac{N_D}{3})^{1/3} e^{-u/2} L^D_{N-1}(u) \Big|_{u=N_D-(4N_D)^{1/3}t} \sim A_i(-t) + O(N_D^{-2/3}).$$

## Section 2. Dirac Density for Harmonic Oscillator with D = 2k+1.

When D is odd, it is possible to get an explicit closed form for the Dirac density.

To do this we refer back to Part II, Section 1.

$$(\mathrm{II}.1.7)\quad \rho_n(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{\alpha^2}{\pi}\right)^{D/2} H_n^D(\alpha(\underset{\sim}{R}+\underset{\sim}{r}),\alpha(\underset{\sim}{R}-\underset{\sim}{r}))e^{-\alpha^2(R^2+r^2)}$$

(density of (n+1)-th "shell")

$$(\mathrm{II}.1.8)\quad \rho^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{\alpha^2}{\pi}\right)^{D/2} \sum_{n=0}^{N-1} H_n^D(\alpha(\underset{\sim}{R}+\underset{\sim}{r}),\alpha(\underset{\sim}{R}-\underset{\sim}{r}))e^{-\alpha^2(R^2+r^2)}$$

and

$$(\mathrm{II}.1.14)\quad \sum_{\ell=1}^{\infty} z^{\ell-1} \sum_{m=0}^{\ell-1} H_m^D(\alpha(\underset{\sim}{R}+\underset{\sim}{r}),\alpha(\underset{\sim}{R}-\underset{\sim}{r}))$$

$$= (1-z)^{-1}(1-z^2)^{-D/2} \exp\left[\frac{2\alpha^2R^2z}{1+z} - \frac{2\alpha^2r^2z}{1-z}\right].$$

For D odd, D = 2k+1, we can write:

$$(\mathrm{II}.2.1)\quad \sum_{m=0}^{\infty} z^m H_m^D(\alpha(\underset{\sim}{R}+\underset{\sim}{r}),\alpha(\underset{\sim}{R}-\underset{\sim}{r}))$$

$$= \frac{(-1)^k}{(2\alpha^2z)^{2k}}\left(\frac{d}{d(R^2)}\right)^k\left(\frac{d}{d(r^2)}\right)^k(1-z^2)^{-1/2}\exp\left[\frac{2\alpha^2R^2\alpha^2}{1+z} - \frac{2\alpha^2r^2z}{1-z}\right]=$$

$$= \frac{(-1)^k}{(2\alpha^2 z)^{2k}} \sum_{m=0}^{\infty} z^m \left(\frac{d}{d(R^2)}\right)^k \left(\frac{d}{d(r^2)}\right)^k \cdot$$

$$\cdot\ H^1_m(\alpha(R+r),\alpha(R-r)) \ .$$

Thus:

$$\text{(II.2.2)}\quad H^{2k+1}_m(\alpha(\underset{\sim}{R}+\underset{\sim}{r}),\alpha(\underset{\sim}{R}-\underset{\sim}{r})) =$$

$$= \frac{(-1)^k}{(2\alpha^2)^{2k}} \left(\frac{d}{d(R^2)}\right)^k \left(\frac{d}{d(r^2)}\right)^k H^1_{m+2k}(\alpha(R+r),\alpha(R-r)) .$$

Also

$$\sum_{\ell=1}^{\infty} z^{\ell-1} \sum_{m=0}^{\ell-1} H^D_m(\alpha(\underset{\sim}{R}+\underset{\sim}{r}),\alpha(\underset{\sim}{R}-\underset{\sim}{r}))$$

$$= \frac{(-1)^{k+1}}{(2\alpha^2 z)^{2k+1}} \left(\frac{d}{d(R^2)}\right)^k \left(\frac{d}{d(r^2)}\right)^{k+1} (1-z^2)^{-1/2} \cdot$$

$$\text{(II.2.3)}\qquad \cdot\ \exp\left[\ \frac{2\alpha^2R^2z}{1+z} - \frac{2\alpha^2r^2z}{1-z}\ \right]$$

$$= \frac{(-1)^{k+1}}{(2\alpha^2 z)^{2k+1}} \left(\frac{d}{d(R^2)}\right)^k \left(\frac{d}{d(r^2)}\right)^{k+1}$$

$$\cdot \sum_{m=0}^{\infty} z^m H^1_m(\alpha(R+r),\alpha(R-r)) .$$

Thus:

$$\text{(II.2.4)}\quad \sum_{m=0}^{\ell-1} H^D_m(\alpha(\underset{\sim}{R}+\underset{\sim}{r}),\alpha(\underset{\sim}{R}-\underset{\sim}{r})) =$$

$$= \frac{(-1)^{k+1}}{(2\alpha^2)^{2k+1}} \left(\frac{d}{d(R^2)}\right)^k \left(\frac{d}{d(r^2)}\right)^{k+1} H^1_{\ell+2k}(\alpha(R+r),\alpha(R-r)) .$$

Thus $\rho_n(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})$, the Dirac density for the (n+1)-th "shell" (that is the sum over the $\binom{n+D-1}{D-1}$ degenerate energy states) for D odd is

$$(\text{II.2.5})\quad \rho_n(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{\alpha^2}{\pi}\right)^{D/2} \frac{(-1)^{\frac{D-1}{2}}}{(2\alpha^2)^{D-1}}\, e^{-\alpha^2(R^2+r^2)}$$

$$\cdot \left(\frac{d}{d(R^2)}\right)^{\frac{D-1}{2}} \left(\frac{d}{d(r^2)}\right)^{\frac{D-1}{2}} \frac{H_{n+D-1}(\alpha(R+r))H_{n+D-1}(\alpha(R-r))}{2^{n+D-1}(n+D-1)!}\,,$$

and

$$(\text{II.2.6})\quad \rho^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{\alpha^2}{\pi}\right)^{D/2} \frac{(-1)^{\frac{D-1}{2}}}{(2\alpha^2)^{D}}\, e^{-\alpha^2(R^2+r^2)}$$

$$\cdot \left(\frac{d}{d(R^2)}\right)^{\frac{D-1}{2}} \left(\frac{d}{d(r^2)}\right)^{\frac{D+1}{2}} \frac{H_{N+D-1}(\alpha(R+r))H_{n+D-1}(\alpha(R-r))}{2^{N+D-1}(N+D-1)!}$$

where $\alpha = \sqrt[4]{mk/\hbar^2}$

and $\rho^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \sum_{n=0}^{N-1} \rho_n(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})$

is the total density of the first N "shells" or, if you prefer, the density of the $\binom{N+D-1}{D}$ lowest states.

## Section 3. The Interacting Harmonic Oscillator.

In this section we will show how a closed form for a one particle density for a system of interacting harmonic oscillators may be obtained by a transformation from the one particle density of a corresponding system of non-interacting oscillators.

The Hamltonian for the interacting system which we will discuss is

$$(\text{II}.3.1)\quad H = \sum_{i=1}^{N_p} \frac{|\underset{\sim}{p}_i|^2}{2m} + \frac{(m\omega^2 - N_p k)}{2} \sum_{i=1}^{N_p} |\underset{\sim}{x}_i|^2 + \frac{k}{4} \sum_{i,j} |\underset{\sim}{x}_i - \underset{\sim}{x}_j|^2$$

or equivalently

$$(\text{II}.3.2)\quad H = \sum_{i=1}^{N_p} \frac{|\underset{\sim}{p}_i|^2}{2m} + \frac{m\omega^2}{2} \sum_{i=1}^{N_p} |\underset{\sim}{x}_i|^2 - \frac{k}{2} \sum_{i,j} \underset{\sim}{x}_i \cdot \underset{\sim}{x}_j$$

The "corresponding" non-interacting system has Hamiltonian:

$$(\text{II}.3.3)\qquad H_0 = \sum_{i=1}^{N_p} \frac{|\underset{\sim}{p}_i|^2}{2m} + \frac{m\omega^2}{2} \sum_{i=1}^{N_p} |\underset{\sim}{x}_i|^2$$

where $\underset{\sim}{p}_i$ and $\underset{\sim}{x}_i$ are vectors of dimension D. $N_p$ is the number of particles in the system.

Transforming to center of mass coordinates:

$$\underset{\sim}{p} = \frac{1}{\sqrt{N_p}} \sum_{i=1}^{N_p} \underset{\sim}{p}_i \qquad \underset{\sim}{x} = \frac{1}{\sqrt{N_p}} \sum_{i=1}^{N_p} \underset{\sim}{x}_i$$

$$\underset{\sim}{p}_i = \underset{\sim}{\bar{p}}_i + \frac{\underset{\sim}{p}}{\sqrt{N_p}} \qquad \underset{\sim}{x}_i = \underset{\sim}{\bar{x}}_i + \frac{\underset{\sim}{x}}{\sqrt{N_p}}$$

then (II.3.1) becomes

$$\text{(II.3.4)} \quad H = \left( \sum_{i=1}^{N_p} \frac{|\underset{\sim}{\bar{p}}_i|^2}{2m} + \frac{m\omega^2}{2} \sum_{i=1}^{N_p} |\underset{\sim}{\bar{x}}_i|^2 \right) + \left( \frac{|\underset{\sim}{p}|^2}{2m} + \frac{m\omega^2 - N_p k}{2} |\underset{\sim}{x}|^2 \right) ;$$

and (II.3.3) becomes

$$\text{(II.3.5)} \quad H_0 = \left( \sum_{i=1}^{N_p} \frac{|\underset{\sim}{\bar{p}}_i|^2}{2m} + \frac{m\omega^2}{2} \sum_{i=1}^{N_p} |\underset{\sim}{\bar{x}}_i|^2 \right) + \left( \frac{|\underset{\sim}{p}_0|^2}{2m} + \frac{m\omega^2}{2} |\underset{\sim}{x}_0|^2 \right) .$$

Now it becomes clear that $H$ and $H_0$ would have the same wave functions if

$$\left( \frac{|\underset{\sim}{p}|^2}{2m} + \frac{m\omega^2 - N_p k}{2} |\underset{\sim}{x}|^2 \right) = \sqrt{\frac{m\omega^2 - N_p k}{m\omega^2}} \left( \frac{|\underset{\sim}{p}_0|^2}{2m} + \frac{m\omega^2}{2} |\underset{\sim}{x}_0|^2 \right) .$$

It can be shown that

$$\text{(II.3.6)} \quad \frac{1}{\sqrt{1 - \frac{N_p k}{m\omega^2}}} \left( \frac{|\underset{\sim}{p}|^2}{2m} + \frac{m\omega^2 - N_p k}{2} |\underset{\sim}{x}|^2 \right) = U \left( \frac{|\underset{\sim}{p}|^2}{2m} + \frac{m\omega^2}{2} |\underset{\sim}{x}|^2 \right) U^{-1}$$

where U is a unitary transformation written in "normally" ordered form:

$$(\text{II.3.7}) \quad U = \beta^{D/2} \exp \frac{-i}{h} [1-\beta] \underset{\sim}{x} \cdot \underset{\sim}{p} \;, \quad \beta = \sqrt[4]{1 - \frac{N_p k}{m\omega^2}} \;.$$

Note!

$$U\, f(\underset{\sim}{x}) = \beta^{D/2} f(\beta\, \underset{\sim}{x})$$

and

$$(\text{II.3.8}) \quad (f,g) = \int f(\underset{\sim}{x})\, g^*(\underset{\sim}{x})\, d\underset{\sim}{x} = \beta^D \int f(\beta\, \underset{\sim}{x})\, g^*(\beta\, \underset{\sim}{x})\, d\underset{\sim}{x}$$

$$= (Uf, Ug) \;.$$

Written in alternate form (II.3.8) becomes

$$\boxed{(\text{II.3.9}) \quad U = \left(\frac{\hbar\, \beta^{1/2}}{2\beta(1-\beta)}\right)^{D} \int e^{\frac{i\hbar}{(1-\beta)} \underset{\sim}{s} \cdot \underset{\sim}{t}}\; e^{i\underset{\sim}{s} \cdot \underset{\sim}{x}}\; e^{i\underset{\sim}{t} \cdot \underset{\sim}{p}}\; d\underset{\sim}{s}\; d\underset{\sim}{t}}$$

where $\beta = \sqrt[4]{1 - \frac{N_p k}{m\omega^2}}$ .

Now since any component of $\underset{\sim}{p}$ or $\underset{\sim}{x}$ commutes with any component of $\underset{\sim}{\bar{p}}_i$ or $\underset{\sim}{\bar{x}}_i$, it becomes clear from (II.3.6) that

$$(\text{II.3.10}) \quad U\, H_0\, U^{-1} = \left( \sum_{i=1}^{N_p} \frac{|\underset{\sim}{\bar{p}}_i|^2}{2m} + \frac{m\omega^2}{2} \sum_{i=1}^{N_p} |\underset{\sim}{\bar{x}}_i|^2 \right)$$

$$+ \frac{1}{\beta^2} \left( \frac{|\underset{\sim}{p}|^2}{2m} + \frac{m\omega^2 - N_p k}{2} |\underset{\sim}{x}|^2 \right).$$

By comparison of (II.3.10) and (II.3.4), we see that although H and $UH_0U^{-1}$ are not the same, they must have the same eigenfunctions.

But $H_0$ defined by (II.3.3) has eigenfunctions of the form:

(II.3.11) $u(\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots, \underset{\sim}{x}_D) =$

$$\cdot \left(\frac{\pi}{\alpha^2}\right)^{\frac{N_p D}{4}} \prod_{i=1}^{N_p} e^{-\frac{1}{2}\alpha^2 |\underset{\sim}{x}_i|^2} \prod_{j=1}^{D} \frac{H_{k_{i,j}}(\alpha\, x_{i\,j})}{[2^{k_{i,j}}(k_{i,j})!]^{1/2}}$$

where $H_{k_{i,j}}(\alpha\, x_{i\,j})$ are the Hermite polynomials used in the last section, $x_{i\,j}$ is the j-th component of $\underset{\sim}{x}_i$ and $\alpha^2 = \frac{m\omega}{h}$. For ease of writing we will define a new set of polynomials in D variables.

$$\text{(II.3.12)} \quad h_n(\underset{\sim}{y}) = \prod_{j=1}^{D} \frac{H_{n_j}(\alpha\, y_j)}{[2^{n_j}(n_j)!]^{1/2}}$$

It is here understood that these polynomials are ordered in some semi-arbitrary fashion $\{h_1(\underset{\sim}{y}), h_2(\underset{\sim}{y}), h_3(\underset{\sim}{y}) \ldots\}$ such that:

First: The indicated sequence exhausts all polynomials of the form (II.3.12) and

Second: Referring to the notation of (II.3.12)

$$\sum_{j=1}^{D} (n+1)_j \geq \sum_{j=1}^{D} n_j \,.$$

Now armed with this new notation we can write down an antisymmetric wave function for $H_0$ of lowest energy.

$$(\text{II.3.13})\quad \psi_0(\underset{\sim}{x}_1,\ldots,\underset{\sim}{x}_{N_p}) = \frac{1}{\sqrt{N_p!}}\left(\frac{\pi}{\alpha^2}\right)^{\frac{N_pD}{4}} e^{-\frac{1}{2}\alpha^2\sum_{i=1}^{N_p}|\underset{\sim}{x}_i|^2}.$$

$$\cdot\begin{vmatrix} h_1(\underset{\sim}{x}_1), & h_2(\underset{\sim}{x}_1),\ldots, & h_N(\underset{\sim}{x}_1) \\ h_1(\underset{\sim}{x}_2) & & \\ \vdots & & \\ h_1(\underset{\sim}{x}_N), & \ldots & h_N(\underset{\sim}{x}_N) \end{vmatrix}$$

But since H has the same functions as $UH_0U^{-1}$ and since the operator U does not disturb the antisymmetry of the wave function, then the wave function $\psi$ for H must be:

$$(\text{II.3.14})\qquad \psi = U\,\psi_0\ .$$

The corresponding one particle Dirac density is:

$$(\text{II.3.15})\quad \rho(\underset{\sim}{x}_1,\underset{\sim}{x}_1') = N_p\int \psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2,\underset{\sim}{x}_3,\ldots,\underset{\sim}{x}_N)\psi^*(\underset{\sim}{x}_1,\underset{\sim}{x}_2,\ldots\underset{\sim}{x}_N)$$

$$\cdot\ d\underset{\sim}{x}_2\ d\underset{\sim}{x}_3\ \ldots\ d\underset{\sim}{x}_N.$$

Combining (II.3.9), (II.3.13) and (II.3.15) we get

$$(\text{II.3.16})\quad \rho(\underset{\sim}{x}_1,\underset{\sim}{x}_1') = \left(\frac{\hbar\beta}{2\pi(1-\beta)}\right)^{1/2\ 2D} \frac{N_p}{N_p!}\left(\frac{\pi}{\alpha^2}\right)^{\frac{ND}{2}}$$

$$\cdot\int d\underset{\sim}{s}\, d\underset{\sim}{t}\, d\underset{\sim}{s}'\, d\underset{\sim}{t}' \Bigg\{ \sum_{i_1\cdot\cdot i_N} \mathcal{E}_{i_1\cdot\cdot i_N} \sum_{j_1\cdot\cdot j_N} \mathcal{E}_{j_1\cdot\cdot j_N}\, e^{\frac{i\hbar}{(1-\beta)}(\underset{\sim}{s}\cdot\underset{\sim}{t}-\underset{\sim}{s}'\cdot\underset{\sim}{t}')}$$

$$\cdot\int \prod_{k=1}^{N} \left(e^{\frac{i\underset{\sim}{s}\cdot\underset{\sim}{x}_k}{\sqrt{N}}}\, e^{\frac{i\underset{\sim}{t}\cdot\underset{\sim}{p}}{\sqrt{N}}}\, e^{-\frac{\alpha^2}{2}|\underset{\sim}{x}_k|^2}\, h_{i_k}(\underset{\sim}{x}_k)\right)$$

$$\cdot\prod_{k'=1}^{N} \left(e^{\frac{i\underset{\sim}{s}'\cdot\underset{\sim}{x}_k'}{\sqrt{N}}}\, e^{\frac{i\underset{\sim}{t}'\cdot\underset{\sim}{p}'}{\sqrt{N}}}\, e^{-\frac{\alpha^2}{2}|\underset{\sim}{x}_{k'}'|^2}\, h_{j_{k'}}(\underset{\sim}{x}_{k'}')\right)^*$$

$$\cdot\ \delta(\underset{\sim}{x}_2-\underset{\sim}{x}_2')\ \delta(\underset{\sim}{x}_3-\underset{\sim}{x}_3')\ \ldots\ \delta(\underset{\sim}{x}_N-\underset{\sim}{x}_N')\ d\underset{\sim}{x}_2\ d\underset{\sim}{x}_2'\ \ldots\ d\underset{\sim}{x}_N\ d\underset{\sim}{x}_N' \Bigg\}$$

but

$$e^{\frac{i\underset{\sim}{t}\cdot\underset{\sim}{p}}{\sqrt{N}}}\, f(\underset{\sim}{x}) = f\left(\underset{\sim}{x} + \frac{\hbar t}{\sqrt{N}}\right)$$

so

$$(\text{II.3.17})\quad \rho(\underset{\sim}{x},\underset{\sim}{x}') = \left(\frac{\hbar\beta}{2\pi(1-\beta)}\right)^{1/2\ 2D} \left(\frac{\pi}{\alpha^2}\right)^{\frac{ND}{2}}$$

$$\cdot\int d\underset{\sim}{s}\ d\underset{\sim}{t}\ d\underset{\sim}{s}'\ d\underset{\sim}{t}'\ e^{\frac{i\hbar}{(1-\beta)}(\underset{\sim}{s}\cdot\underset{\sim}{t}-\underset{\sim}{s}'\cdot\underset{\sim}{t}')}\ I(\underset{\sim}{x},\underset{\sim}{x}':\underset{\sim}{s},\underset{\sim}{t},\underset{\sim}{s}',\underset{\sim}{t}')$$

where

$$(\text{II}.3.18)\quad I(\underset{\sim}{x}_1,\underset{\sim}{x}_1':\underset{\sim}{s},\underset{\sim}{t},\underset{\sim}{s}',\underset{\sim}{t}') = \frac{1}{(N-1)!}\int [d\underset{\sim}{x}_2 d\underset{\sim}{x}_2' d\underset{\sim}{x}_3 d\underset{\sim}{x}_3' \ldots d\underset{\sim}{x}_N d\underset{\sim}{x}_N'$$

$$\delta(\underset{\sim}{x}_2-\underset{\sim}{x}_2')\delta(\underset{\sim}{x}_3-\underset{\sim}{x}_3') \ldots \delta(\underset{\sim}{x}_N-\underset{\sim}{x}_N')$$

$$\cdot \sum_{i_1\cdots i_N} \mathcal{E}_{\underset{\sim}{i}} \sum_{j_1\cdots j_N} \mathcal{E}_{\underset{\sim}{j}} \prod_{k=1}^{N} (e^{\frac{i\underset{\sim}{s}\cdot\underset{\sim}{x}_k}{\sqrt{N}}} e^{-\frac{\alpha^2}{2}|\underset{\sim}{x}_k+\frac{\hbar\underset{\sim}{t}}{\sqrt{N}}|^2} h_{i_k}(\underset{\sim}{x}_k+\frac{\hbar\underset{\sim}{t}}{\sqrt{N}}))$$

$$\cdot \prod_{k'=1}^{N} (e^{\frac{-i\underset{\sim}{s}'\cdot\underset{\sim}{x}_k'}{\sqrt{N}}} e^{-\frac{\alpha^2}{2}|\underset{\sim}{x}_{k'}'+\frac{\hbar\underset{\sim}{t}'}{\sqrt{N}}|^2} h_{j_{k'}}(\underset{\sim}{x}_{k'}'+\frac{\hbar\underset{\sim}{t}'}{\sqrt{N}}))\ ].$$

Now it is clear that by adding and subtracting columns:

$$\begin{vmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^N \\ 1 & x_2 & x_2^2 & \ldots & x_2^N \\ \vdots & & & & \\ 1 & x_N & x_N^2 & \ldots & x_N^N \end{vmatrix} = \begin{vmatrix} 1 & (x_1-a) & (x_1-a)^2 & \ldots & (x_1-a)^N \\ 1 & (x_2-a) & (x_2-a)^2 & \ldots & (x_2-a)^N \\ \vdots & & & & \\ 1 & (x_N-a) & (x_N-a)^2 & \ldots & (x_N-a)^N \end{vmatrix}$$

It is also clear that this can be generalized to Hermite polynomials, and then generalized again to the $h_n(\underset{\sim}{x})$ polynomials. Thus:

$$(\text{II}.3.19)\quad \sum_{i_1\ldots i_N} \mathcal{E}_{\underset{\sim}{i}} \prod_{k=1}^{N} e^{\frac{i\underset{\sim}{s}\cdot\underset{\sim}{x}_k}{\sqrt{N}}} e^{-\frac{\alpha^2}{2}|\underset{\sim}{x}_k+\frac{\hbar\underset{\sim}{t}}{\sqrt{N}}|^2} h_{i_k}(\underset{\sim}{x}_k+\frac{\hbar\underset{\sim}{t}}{\sqrt{N}})$$

$$= \sum_{i_1\ldots i_N} \mathcal{E}_{\underset{\sim}{i}} \prod_{k=1}^{N} e^{\frac{i s\cdot x_k}{\sqrt{N}}} e^{-\frac{\alpha^2}{2}|\underset{\sim}{x}_k+\frac{\hbar\underset{\sim}{t}}{\sqrt{N}}|} h_{i_k}(\underset{\sim}{x}_k+\frac{\hbar}{2\sqrt{N}}(\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i}{m\omega}(\underset{\sim}{s}-\underset{\sim}{s}')))$$

Continuing along this line and using the fact that

$$(\text{II}.3.20)\quad \left(e^{-\frac{\alpha^2}{2}\left|\underset{\sim}{x}_k+\frac{\hbar\underset{\sim}{t}}{\sqrt{N}}\right|^2} e^{\frac{i\underset{\sim}{s}\cdot\underset{\sim}{x}_k}{\sqrt{N}}}\right)\cdot\left(e^{-\frac{\alpha^2}{2}\left|x_k+\frac{\hbar\underset{\sim}{t}'}{\sqrt{N}}\right|^2} e^{\frac{-i\underset{\sim}{s}'\cdot\underset{\sim}{x}_k}{\sqrt{N}}}\right)$$

$$= e^{-\alpha^2\left|\underset{\sim}{x}_k+\frac{\hbar}{2\sqrt{N}}\left(\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i\underset{\sim}{s}}{m\omega}+\frac{i\underset{\sim}{s}'}{m\omega}\right)\right|^2} e^{\frac{\alpha^2\hbar^2}{4N}\left|\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i}{m\omega}(\underset{\sim}{s}-\underset{\sim}{s}')\right|^2}$$

$$\cdot\, e^{\frac{-\alpha^2\hbar^2}{2N}\left(|\underset{\sim}{t}|^2+|\underset{\sim}{t}'|^2\right)}$$

and the fact that:

$$(\text{II}.3.21)\quad \int d\underset{\sim}{u}\; e^{-\alpha^2\left|\underset{\sim}{u}+\frac{\hbar}{2\sqrt{N}}\left(\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i\underset{\sim}{s}}{m\omega}+\frac{i\underset{\sim}{s}'}{m\omega}\right)\right|^2}$$

$$\cdot\, h_i\!\left(\underset{\sim}{u}+\frac{\hbar}{2\sqrt{N}}\left(\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i\underset{\sim}{s}}{m\omega}+\frac{i\underset{\sim}{s}'}{m\omega}\right)\right) h_j\!\left(\underset{\sim}{u}+\frac{\hbar}{2\sqrt{N}}\left(\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i\underset{\sim}{s}}{m\omega}+\frac{i\underset{\sim}{s}'}{m\omega}\right)\right)$$

$$= \delta_{ij}\left(\frac{\alpha^2}{\pi}\right)^{D/2}$$

We get from (II.3.18)

$$(\text{II}.3.22)\quad I = \left(\frac{\alpha^2}{\pi}\right)^{\frac{D(N-1)}{2}} e^{\frac{\alpha^2\hbar^2}{4N}(N-1)\left|\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i}{m\omega}(\underset{\sim}{s}-\underset{\sim}{s}')\right|^2}$$

$$\cdot\, e^{\frac{-\alpha^2\hbar^2}{2N}(N-1)\left(|\underset{\sim}{t}|^2+|\underset{\sim}{t}'|^2\right)} \left(e^{-\frac{\alpha^2}{2}\left|\underset{\sim}{x}_1+\frac{\hbar\underset{\sim}{t}}{\sqrt{N}}\right|^2} e^{\frac{i\underset{\sim}{s}\cdot\underset{\sim}{x}_1}{\sqrt{N}}}\; e^{-\frac{\alpha^2}{2}\left|\underset{\sim}{x}_1'+\frac{\hbar\underset{\sim}{t}'}{\sqrt{N}}\right|^2} e^{\frac{-i\underset{\sim}{s}'\cdot\underset{\sim}{x}_1'}{\sqrt{N}}}\right)$$

$$\cdot\sum_{i=1}^{N} h_i\!\left(\underset{\sim}{x}_1+\frac{\hbar}{2\sqrt{N}}\left(\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i\underset{\sim}{s}}{m\omega}+\frac{i\underset{\sim}{s}'}{m\omega}\right)\right) h_i\!\left(\underset{\sim}{x}_1'+\frac{\hbar}{2\sqrt{N}}\left(\underset{\sim}{t}+\underset{\sim}{t}'-\frac{i\underset{\sim}{s}}{m\omega}+\frac{i\underset{\sim}{s}'}{m\omega}\right)\right)$$

Now let us substitute

$$\underset{\sim}{\mathcal{T}} = \frac{\underset{\sim}{t} + \underset{\sim}{t}'}{2} \qquad \underset{\sim}{\mathcal{S}} = \frac{\underset{\sim}{s} - \underset{\sim}{s}'}{2}$$

$$\underset{\sim}{\mathscr{t}} = \underset{\sim}{t} - \underset{\sim}{t}' \qquad \underset{\sim}{\mathscr{s}} = \underset{\sim}{s} + \underset{\sim}{s}'$$

Combining (II.3.22) and (II.3.17) with the new variables we get

$$\text{(II.3.23)} \quad \rho(\underset{\sim}{x},\underset{\sim}{x}') = \left(\frac{\hbar\,\beta^{1/2}}{2\pi(1-\beta)}\right)^{2D} \left(\frac{\pi}{\alpha^2}\right)^{D/2} \int d\underset{\sim}{\mathscr{s}}\, d\underset{\sim}{\mathcal{S}}\, d\underset{\sim}{\mathscr{t}}\, d\underset{\sim}{\mathcal{T}}$$

$$\cdot \Bigg| e^{\frac{i\hbar}{(1-\beta)}\left(\frac{\underset{\sim}{\mathscr{s}}\cdot\underset{\sim}{\mathscr{t}}}{2}\right) + 2\underset{\sim}{\mathcal{S}}\cdot\underset{\sim}{\mathcal{T}})} \; e^{\frac{\alpha^2\hbar^2}{N}(N-1)\left|\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}\right|^2} \; e^{-\alpha^2\hbar^2\left(\frac{|\underset{\sim}{\mathscr{t}}|^2}{4} + |\mathcal{T}|^2\right)}$$

$$\cdot\; e^{-\frac{\alpha^2}{2}\left(|\underset{\sim}{x}|^2 + |\underset{\sim}{x}'|^2\right)} \; e^{\frac{-\alpha^2 h}{2\sqrt{N_p}}\underset{\sim}{\mathscr{t}}\cdot(\underset{\sim}{x}-\underset{\sim}{x}')} \; e^{\frac{\alpha^2\hbar}{\sqrt{N_p}}\underset{\sim}{\mathcal{T}}\cdot(\underset{\sim}{x}+\underset{\sim}{x}')}$$

$$\cdot\; e^{\frac{i\underset{\sim}{\mathcal{S}}}{\sqrt{N}}\cdot(\underset{\sim}{x}+\underset{\sim}{x}')} \; e^{\frac{i\underset{\sim}{\mathscr{s}}}{2\sqrt{N}}\cdot(\underset{\sim}{x}-\underset{\sim}{x}')}$$

$$\cdot \sum_{i=1}^{N} h_i\left(\underset{\sim}{x} + \frac{\hbar}{\sqrt{N_p}}\left(\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}\right)\right) h_i\left(\underset{\sim}{x}' + \frac{\hbar}{\sqrt{N_p}}\left(\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}\right)\right.\Bigg| ,$$

where $\left|\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}\right|^2 = \left(\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}\right)\cdot\left(\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}\right)$ .

The variables $\underset{\sim}{s}$ and $\underset{\sim}{t}$ may be integrated immediately giving us:

$$(\text{II.3.24})\quad \rho(\underset{\sim}{x},\underset{\sim}{x}') = \left(\frac{\hbar\,\beta}{\pi^{1/2}\alpha\,|1-\beta|}\right)^{D} \exp\left[\frac{\alpha^{2}(1-\beta^{2})\,|\underset{\sim}{x}-\underset{\sim}{x}'|^{2}}{4N_{p}}\right]$$

$$\cdot \int d\underset{\sim}{\mathcal{S}}\; d\underset{\sim}{\mathcal{T}}\, [\exp\left(\frac{2ih}{(1-\beta)}\underset{\sim}{\mathcal{S}}\cdot\underset{\sim}{\mathcal{T}} + \frac{\alpha^{2}h^{2}}{N_{p}}(N_{p}-1)\,|\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}|^{2}\right.$$

$$- \alpha^{2}h^{2}|\underset{\sim}{\mathcal{T}}|^{2} - \frac{\alpha^{2}}{2}\left(|\underset{\sim}{x}|^{2} + |\underset{\sim}{x}'|^{2}\right) + \frac{\alpha^{2}\hbar}{\sqrt{N_{p}}}\,\underset{\sim}{\mathcal{T}}\cdot(\underset{\sim}{x}+\underset{\sim}{x}')$$

$$\left. + \frac{i\underset{\sim}{\mathcal{S}}}{N_{p}}\cdot(\underset{\sim}{x}+\underset{\sim}{x}')\right)\cdot \sum_{i=1}^{N_{p}} h_{i}\left(\underset{\sim}{x}+\frac{\hbar}{\sqrt{N_{p}}}\left(\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}\right)\right) h_{i}\left(\underset{\sim}{x}'+\frac{\hbar}{\sqrt{N_{p}}}\left(\underset{\sim}{\mathcal{T}} - \frac{i}{m\omega}\underset{\sim}{\mathcal{S}}\right)\right)$$

Now substituting:

$$\underset{\sim}{x} = \underset{\sim}{R} + \underset{\sim}{r}$$

$$\underset{\sim}{x}' = \underset{\sim}{R} - \underset{\sim}{r}$$

$$\underset{\sim}{\mathcal{T}} = \frac{\sqrt{N_{p}}}{\hbar}\,(\underset{\sim}{v} - \underset{\sim}{R})$$

$$\underset{\sim}{\mathcal{S}} = \alpha^{2}\sqrt{N_{p}}\;\underset{\sim}{u}$$

and using the fact that

$$\rho_{0}(\underset{\sim}{x},\underset{\sim}{x}') = \left(\frac{\pi}{\alpha^{2}}\right)^{D/2} e^{-\frac{\alpha^{2}}{2}\left(|\underset{\sim}{x}|^{2}+|\underset{\sim}{x}'|^{2}\right)} \sum_{i=1}^{N_{p}} h_{i}(\underset{\sim}{x})\; h_{i}(\underset{\sim}{x}')$$

we finally arrive at the equation:

$$\boxed{\begin{aligned}&(\text{II.3.25})\quad \rho(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{N_p\alpha^2\beta}{\pi|1-\beta|}\right)^D e^{\frac{\alpha^2(1-\beta^2)|\underset{\sim}{r}|^2}{N_p}}\\[2ex]
&\cdot \iint d\underset{\sim}{u}\, d\underset{\sim}{v}\, \exp\left[-N_p\alpha^2|\underset{\sim}{u}|^2 + \frac{2iN_p\alpha^2\beta}{(1-\beta)}\,\underset{\sim}{u}\cdot\underset{\sim}{v} - \frac{2iN_p\alpha^2\beta}{(1-\beta)}\,\underset{\sim}{u}\cdot\underset{\sim}{R}\right]\\[2ex]
&\cdot\rho_0(\underset{\sim}{v}-i\underset{\sim}{u}+\underset{\sim}{r},\ \underset{\sim}{v}-i\underset{\sim}{u}-\underset{\sim}{r})\end{aligned}}$$

In the special cases that $N_p = \binom{D-1+N}{D}$, $N = 1,2,\ldots,$ we have a closed shell structure and we may obtain a more explicit form for $\rho(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})$.

Following the notation of Section 2, we will denote such a density by $\rho^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})$.

Now from equation (II.1.16)

$$\sum_{N=1}^{\infty} z^{N-1}\rho_0^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})$$

$$= \left(\frac{\alpha^2}{\pi}\right)^{D/2}(1-z)^{-\frac{(D+2)}{2}}(1+z)^{-D/2}\exp\left[-\frac{\alpha^2R^2(1-z)}{1+z} - \frac{\alpha^2r^2(1+z)}{1-z}\right]$$

Thus

$$(\text{II.3.26})\quad \sum_{N=1}^{\infty} z^{N-1}\,\rho^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})$$

$$= \left(\frac{\alpha^2}{\pi}\right)(1-z)^{-\left(\frac{D+2}{2}\right)}(1+z)^{-D/2}\left(\frac{N_p\alpha^2\beta}{\pi|1-\beta|}\right)^D\exp\left[\frac{\alpha^2(1-\beta^2)|\underset{\sim}{r}|^2}{N_p}\right]$$

$$\cdot\iint d\underset{\sim}{u}\, d\underset{\sim}{v}\,\exp\left[-N_p\alpha^2|\underset{\sim}{u}|^2 + \frac{2iN_p\alpha^2\beta}{(1-\beta)}\,\underset{\sim}{u}\cdot\underset{\sim}{v} - \frac{2iN_p\alpha^2\beta}{(1-\beta)}\,\underset{\sim}{u}\cdot\underset{\sim}{R}\right]$$

$$\cdot\exp\left[-\frac{\alpha^2(1-z)}{(1+z)}\left(|\underset{\sim}{v}|^2 - 2i\underset{\sim}{u}\cdot\underset{\sim}{v} - |\underset{\sim}{u}|^2\right) - \frac{\alpha^2(1+z)}{(1-z)}|\underset{\sim}{r}|^2\right].$$

Carrying out the indicated integrations we arrive at the equation:

$$(\mathrm{II.3.27})\quad \sum_{N=1}^{\infty} z^{N-1}\rho^{N}(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{\alpha^2}{\pi}\right)^{D/2} \left(\frac{N_p\beta^2}{N_p\beta^2-\beta^2+1}\right)^{D/2} \cdot$$

$$\cdot \exp\left[-\frac{\alpha^2(\beta^2-1)}{N_p} r^2\right] \exp\left[-\alpha^2\left(\frac{N_p\beta^2}{N_p\beta^2-\beta^2+1}\right)R^2 - \alpha^2 r^2\right]$$

$$\cdot \left\{ (1-z)^{-\frac{D+2}{2}} \left(1+\frac{N_p\beta^2+\beta^2-1}{N_p\beta^2-\beta^2+1}z\right)^{-D/2} \right.$$

$$\left. \cdot \exp\left| \frac{\frac{2N_p^2\alpha^2\beta^4R^2}{N_p^2\beta^4-(1-\beta^2)^2}\left(\frac{N_p\beta^2+\beta^2-1}{N_p\beta^2-\beta^2+1}z\right)}{1+\left(\frac{N_p\beta^2+\beta^2-1}{N_p\beta^2-\beta^2+1}\right)z} - \frac{2\alpha^2 z r^2}{(1-z)} \right| \right\}$$

where we have substituted $R = |\underset{\sim}{R}|$ and $r = |\underset{\sim}{r}|$.

Now if we substitute $\gamma = \frac{\beta^2-1}{N_p\beta^2}$ and expand the part of the last equation within $\{\ \}$ in terms of Laguerre polynomials and then we get:

$$(\mathrm{II.3.28})\quad \sum_{N=1}^{\infty} z^{N-1}\rho^{N}(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) =$$

$$= \left(\frac{\alpha^2}{\pi}\right)^{D/2} \left(\frac{1}{1-\gamma}\right)^{D/2} \exp\left[-\frac{\alpha^2\gamma}{1-N\gamma} r^2\right] \exp\left[-\frac{\alpha^2R^2}{(1-\gamma)} - \alpha^2 r^2\right]$$

$$\cdot \left\{ \left(\sum_{\ell=0}^{\infty} z^{\ell} L_{\ell}^{D/2}(2\alpha^2r^2)\right) \left(\sum_{m=0}^{\infty} (-z)^m\left(\frac{1+\gamma}{1-\gamma}\right)^m L_m^{\frac{D-2}{2}}\left(\frac{2\alpha^2R^2}{1-\gamma^2}\right)\right) \right\}.$$

Thus for the Hamiltonian,

$$H = \sum_{i=1}^{N_p} \frac{|\underset{\sim}{p}_i|^2}{2m} + \frac{k_0}{2} \sum_{i=1}^{N_p} |\underset{\sim}{x}_i|^2 + \frac{k}{4} \sum_{i,j} |\underset{\sim}{x}_i - \underset{\sim}{x}_j|^2$$

we have arrived at the Dirac density $\rho^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r})$ where $N_p\binom{D-1+N}{D}$

$$\boxed{\begin{aligned}&(\text{II.3.39})\ \rho^N(\underset{\sim}{R}+\underset{\sim}{r},\underset{\sim}{R}-\underset{\sim}{r}) = \left(\frac{\alpha^2}{\pi}\right)^{D/2} (1-\gamma)^{-D/2} \\ &\cdot \exp\left[ -\frac{\alpha^2 R^2}{(1-\gamma)} - \frac{\alpha^2(1-(N-1)\gamma)}{(1-N\gamma)}\, r^2 \right] \\ &\cdot \sum_{m=0}^{N-1} (-1)^m \left(\frac{1+\gamma}{1-\gamma}\right)^m L_m^{\frac{D-2}{2}}\left(\frac{2\alpha^2 R^2}{1-\gamma^2}\right) L_{N-1-m}^{D/2}(2\alpha^2 r^2)\end{aligned}}$$

where $\gamma = \dfrac{1 - \sqrt{1 + \frac{N_p k}{k_0}}}{N_p}$ and $\alpha^2 = \dfrac{\sqrt{mk_0}}{\hbar} \sqrt{1 + \dfrac{N_p k}{k_0}}$ .

To conclude this discussion of the exact solution for the interacting harmonic oscillator, we will consider the lowest energy level.

Rewriting equations (II.3.4) and (II.3.5)

$$(\text{II.3.4})\ H = \left( \sum_{i=1}^{N_p} \frac{|\bar{\underset{\sim}{p}}_i|^2}{2m} + \frac{m\omega^2}{2} \sum_{i=1}^{N_p} |\bar{\underset{\sim}{x}}_i|^2 \right) + \left( \frac{|\underset{\sim}{p}|^2}{2m} + \frac{m\omega^2 - N_p k}{2} |\underset{\sim}{x}|^2 \right)$$

$$(\text{II.3.5})\ H_0 = \left( \sum_{i=1}^{N_p} \frac{|\bar{\underset{\sim}{p}}_i|^2}{2m} + \frac{m\omega^2}{2} \sum_{i=1}^{N_p} |\bar{\underset{\sim}{x}}_i|^2 \right) + \left( \frac{|\underset{\sim}{p}_0|^2}{2m} + \frac{m\omega^2}{2} |\underset{\sim}{x}_0|^2 \right).$$

Examining these two equations we see that difference in energies arises from the second terms thus

$$E - E_0 = \frac{D}{2}\hbar \left[ \sqrt{\omega^2 - \frac{N_p k}{m}} - \omega \right]$$

or

$$E - E_0 = \frac{D}{2}\hbar \left[ \sqrt{\frac{k_0}{m}} - \sqrt{\frac{k_0 + N_p k}{m}} \right] .$$

For the closed shell system $N_p = \binom{D-1+N}{D}$. It can be shown that after summing over all degeneracies that for the total energy $E_0$ for the non-interacting system (II.3.5) we may write

$$E_0 = \frac{D(D-1+2N)}{2(D+1)} \binom{D-1+N}{D} \hbar\omega$$

Thus for the Hamiltonian:

$$H = \sum_{i=1}^{N_p} \frac{|\underset{\sim}{p}_i|^2}{2m} + \frac{k_0}{2} \sum_{i=1}^{N_p} |\underset{\sim}{x}_i|^2 + \frac{k}{4} \sum_{i,j} |\underset{\sim}{x}_i - \underset{\sim}{x}_j|^2$$

the lowest total energy

$$E = \frac{D(D-1+2N)}{2(D+1)} \binom{D-1+N}{D} \hbar \sqrt{\frac{k_0 + N_p k}{m}} + \frac{D}{2}\hbar \left[ \sqrt{\frac{k_0}{m}} - \sqrt{\frac{k_0 + N_p k}{m}} \right]$$

## Section 4. The Hartree-Fock Solution Minus the Exchange Term for the D Dimensional, $N_p$ Particle Interacting Harmonic Oscillator.

Consider the Hamiltonian

$$(\text{II.4.1})\quad H = \sum_{i=1}^{N_p} -\frac{\hbar^2}{2m}\nabla^2_{\underset{\sim}{x}_i} + \frac{k_0}{2}\sum_{j=1}^{N_p} |\underset{\sim}{x}_i|^2 + \frac{k}{4}\sum_{i,j} |\underset{\sim}{x}_i - \underset{\sim}{x}_j|$$

where $\underset{\sim}{x}_i = (x_{i1}, x_{i2}, \ldots, x_{iD})$

and $\nabla^2_{\underset{\sim}{x}_i} = \sum_{m=1}^{D} \frac{\partial^2}{\partial x_{im}^2}$ .

Let us rewrite (II.4.1) in the form:

$$(\text{II.4.2})\quad H = \sum_{i=1}^{N_p} -\frac{\hbar^2}{2m}\nabla^2_{\underset{\sim}{x}_i} + \frac{k_0+(N_p-1)k}{2}\sum_{i=1}^{N_p} |\underset{\sim}{x}_i|^2 - k\sum_{\substack{i,j\\ i>j}} \underset{\sim}{x}_i \cdot \underset{\sim}{x}_j .$$

Suppose we make the Hartree-Fock approximation that

$$\psi(\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots, \underset{\sim}{x}_p) = \frac{1}{\sqrt{N_p!}} \begin{vmatrix} \psi_1(\underset{\sim}{x}_1), & \psi_1(\underset{\sim}{x}_2)\ , & \ldots & \psi_1(\underset{\sim}{x}_{N_p}) \\ \psi_2(\underset{\sim}{x}_1) & & & \\ \ldots & & & \\ \psi_{N_p}(\underset{\sim}{x}_1) & & & \psi_{N_p}(\underset{\sim}{x}_{N_p}) \end{vmatrix}$$

then

$$(\text{II.4.3})\langle H\rangle = -\frac{\hbar^2}{2m}\sum_{i=1} \int \psi_i^*(\underset{\sim}{x})\ \nabla^2_{\underset{\sim}{x}}\ \psi_i(\underset{\sim}{x})\ d\underset{\sim}{x}$$

$$+ \frac{k_0+(N_p-1)k}{2}\sum_{i} \int \psi_i^*(\underset{\sim}{x})\ |\underset{\sim}{x}|^2\ \psi_i(\underset{\sim}{x})\ d\underset{\sim}{x}\ -$$

$$- k \sum_{\substack{i,j\\ i>j}} \int \psi_i^*(\underset{\sim}{x})\, \psi_j^*(\underset{\sim}{x}')\underset{\sim}{x}\cdot\underset{\sim}{x}' \,(\psi_i(\underset{\sim}{x})\psi_j(\underset{\sim}{x}')-\psi_i(\underset{\sim}{x}')\psi_j(\underline{x}))\, d\underset{\sim}{x}\, d\underset{\sim}{x}'$$

Now:

$$\delta(\langle H\rangle + \sum_{i,j} \lambda_{ij} \int \psi_i^*(x)\, \psi_j(\underset{\sim}{x})\, d\underset{\sim}{x}\ ) = 0 \ .$$

And since the coefficient of $\delta\psi_i^*(\underset{\sim}{x})$ is equal to zero, we may write

$$\text{(II.4.4)} \quad - \frac{\hbar^2}{2m} \nabla^2_{\underset{\sim}{x}}\ \psi_i(\underset{\sim}{x}) + \frac{k_0+(N_p-1)k}{2} |\underset{\sim}{x}\nabla|^2 \psi_i(\underset{\sim}{x})$$

$$- k \int \rho(\underset{\sim}{x}',\underset{\sim}{x}')\underset{\sim}{x}\cdot\underset{\sim}{x}'\, d\underset{\sim}{x}'\ \psi_i(\underset{\sim}{x}) + k \int \rho(\underset{\sim}{x},\underset{\sim}{x}')\underset{\sim}{x}\cdot\underset{\sim}{x}'\ \psi_i(\underset{\sim}{x}')d\underset{\sim}{x}'$$

$$= \sum_j \lambda_{i,j}\ \psi_j(\underset{\sim}{x}) \ .$$

Since $(\lambda_{i,j})$ is a Hermitian matrix, it may be diagonalized by a unitary transformation $(U_{ij})$ that will give us a new set of orbital functions

$$u_i(x) = \sum_j U_{i,j}\ \psi_j(\underset{\sim}{x})$$

$$\varepsilon_i = \sum_{k,j} U_{i,k}\lambda_{k,j}\ U^*_{i,j} \ .$$

We then get the new set of equations

$$(\mathrm{II}.4.5)\quad -\frac{\hbar^2}{2m}\nabla^2_{\underset{\sim}{x}}\, u_i(\underset{\sim}{x}) + \frac{k_0+(N_p-1)k}{2}\,|\underset{\sim}{x}|^2\, u_i(\underset{\sim}{x})$$

$$- k\int \rho(\underset{\sim}{x}',\underset{\sim}{x}')\underset{\sim}{x}\cdot\underset{\sim}{x}'\, d\underset{\sim}{x}'\, u_i(\underset{\sim}{x}) + k\int \rho(\underset{\sim}{x},\underset{\sim}{x}')\underset{\sim}{x}\cdot\underset{\sim}{x}'\, u_i(\underset{\sim}{x}')d\underset{\sim}{x}'$$

$$= \varepsilon_i u_i(\underset{\sim}{x})$$

where $\rho(\underset{\sim}{x},\underset{\sim}{x}') = \sum_i \psi_i(\underset{\sim}{x})\,\psi_i^*(\underset{\sim}{x}') = \sum_i u_i(\underset{\sim}{x})\,u_i^*(\underset{\sim}{x}')$.

However $\int \rho(\underset{\sim}{x}',\underset{\sim}{x}')\underset{\sim}{x}\cdot\underset{\sim}{x}'\, d\underset{\sim}{x}' = 0$ ,

and the last term on the left hand side of (II.4.5) is the contribution from the exchange term which we here choose to ignore.

We are thus left with the equation

$$-\frac{\hbar^2}{2m}\nabla^2_{\underset{\sim}{x}}\, u_i(\underset{\sim}{x}) + \frac{k_0+(N_p-1)k}{2}\,|\underset{\sim}{x}|^2\, u_i(\underset{\sim}{x}) = \varepsilon_i\, u_i(\underset{\sim}{x}) .$$

We thus get the usual eigenvalues

$$\varepsilon_i = (n_i + \frac{D}{2})\,\hbar\sqrt{\frac{k_0+(N_p-1)k}{m}}$$

with a degeneracy of $\binom{n_i+D-1}{D-1}$.

If we continue to ignore the exchange term

$$\langle H\rangle \approx \sum_{i=1}^{N_p} \varepsilon_i .$$

For N "shells" we have

$$\sum_{n_i=0}^{N-1} \binom{n_i+D-1}{D-1} = \binom{N+D-1}{D} \text{ different orbitals}$$

thus if $N_p = \binom{N+D-1}{D}$ , $N = 1,2,\ldots,$ we may write

$$\langle H \rangle \approx \sum_{n_i=0}^{N-1} \binom{n_i+D-1}{D-1} \left(n_i + \frac{D}{2}\right) \hbar \sqrt{\frac{k_0+(N_p-1)k}{m}}$$

or

$$\text{(II.4.6)} \quad \langle H \rangle \approx \frac{D(D-1+2N)}{2(D+1)} \binom{D-1+N}{D} \hbar \sqrt{\frac{k_0+(N_p-1)k}{m}}$$

For comparison let us write the exact energy from page 59:

$$\langle H \rangle = \frac{D(D-1+2N)}{2(D+1)} \binom{D-1+N}{D} \hbar \sqrt{\frac{k_0+N_p k}{m}} + \frac{D}{2} \hbar \left[ \sqrt{\frac{k_0}{m}} - \sqrt{\frac{k_0+N_p k}{m}} \right]$$

## Section 5. The Thomas Fermi Approximation for the Interacting Harmonic Oscillator.

The Wigner-Moyal density without the spin factor of 2 for the Thomas-Fermi approximation is:

$$\rho(\underset{\sim}{p},\underset{\sim}{r}) = \frac{1}{h^D} \Theta \left(E - V(\underset{\sim}{r}) - \frac{p^2}{2m}\right) .$$

Thus

$$\text{(II.5.1)} \quad t(\underset{\sim}{r}) = \Omega_D \int_0^{\infty} \frac{p^2}{2m} \rho(\underset{\sim}{p},\underset{\sim}{r})\, p^{D-1}\, dp = \frac{\Omega_D}{h^D 2m} \frac{[2m(E-V)]^{\frac{D+2}{2}}}{D+2} .$$

On the other hand

$$(\text{II.5.2})\quad \rho(\underset{\sim}{r}) = \Omega_D \int_0^\infty \rho(\underset{\sim}{p},\underset{\sim}{r})\, p^{D-1}\, dp = \frac{\Omega_D}{h^D}\, \frac{[2m(E-V)]^{D/2}}{D} .$$

We thus arrive at the approximation

$$(\text{II.5.3})\quad t(\underset{\sim}{r}) = \frac{h^2}{2m}\, \frac{D^{\frac{D+2}{D}}}{(\Omega_D)^{2/D}\,(D+2)}\, [\rho(\underset{\sim}{r})]^{\frac{D+2}{D}} .$$

The Hamiltonian used in the last section was

$$(\text{II.5.4})\quad H = \sum_{i=1}^{N_p} \frac{|\underset{\sim}{p}_i|^2}{2m} + \frac{k_0+(N_p-1)k}{2} \sum_i |\underset{\sim}{x}_i|^2 - k \sum_{\substack{i,j\\ i>j}} \underset{\sim}{x}_i \cdot \underset{\sim}{x}_j .$$

Now using approximation (II.5.3) we find that the total energy of the system

$$(\text{II.5.5})\quad \langle H \rangle = \frac{h^2}{2m}\, \frac{D^{\frac{D+2}{D}}}{(\Omega_D)^{2/D}(D+2)} \int [\rho(\underset{\sim}{x})]^{\frac{D+2}{D}} d\underset{\sim}{x}$$

$$+ \frac{k_0+(N_p-1)k}{2} \int |\underset{\sim}{x}|^2 \rho(\underset{\sim}{x})\, d\underset{\sim}{x}$$

$$- \frac{k}{2} \int \underset{\sim}{x}\cdot\underset{\sim}{x}'[\rho(\underset{\sim}{x},\underset{\sim}{x})\rho(\underset{\sim}{x}',\underset{\sim}{x}')-\rho(\underset{\sim}{x},\underset{\sim}{x}')\rho(\underset{\sim}{x}',\underset{\sim}{x})]d\underset{\sim}{x}'d\underset{\sim}{x}$$

Now $\int \underset{\sim}{x}\cdot\underset{\sim}{x}'\rho(\underset{\sim}{x},\underset{\sim}{x})\, d\underset{\sim}{x} = 0$

and we will ignore the exchange term as we did in the last section. This gives us

$$(\text{II.5.6})\ \langle H\rangle = \frac{h^2}{2m}\ \frac{D^{\frac{D+2}{D}}}{(\Omega_D)^{2/D}(D+2)} \int [\rho(\underset{\sim}{x})]^{\frac{D+2}{D}}\ d\underset{\sim}{x}$$

$$+ \frac{k_0+(N_p-1)k}{2} \int |\underset{\sim}{x}|^2\ \rho(\underset{\sim}{x})\ d\underset{\sim}{x}\ .$$

Using the relation that

$$\delta(\langle H\rangle - E \int \rho(\underset{\sim}{x})\ d\underset{\sim}{x}) = 0\ ,$$

we obtain the equation

$$\frac{h^2}{2m}\ \frac{D^{2/D}}{(\Omega_D)^{2/D}} [\rho(\underset{\sim}{x})]^{2/D} + \frac{k_0+(N_p-1)k}{2} |\underset{\sim}{x}|^2 - E = 0$$

or

$$(\text{II.5.7})\quad \rho(\underset{\sim}{x}) = \frac{\Omega_D}{h^D D} [2m(E - \frac{k_0+(N_p-1)k}{2} |\underset{\sim}{x}|^2)]^{D/2}.$$

We can obtain E from the equation

$$\Omega_D \int_0^\infty \rho(\underset{\sim}{x})\ x^{D-1}\ dx = N_p$$

$$N_p = \frac{(\Omega_D)^2[2m]^{D/2}}{h^D D} \int_0^{\sqrt{E/A}} [E - Ax^2]^{D/2}\ x^{D-1}\ dx$$

where $A = \frac{k_0+(N_p-1)k}{2}$ .

If we substitute

$$x = \sqrt{\frac{E}{A}}\ \sin\theta$$

we get

$$N_p = \frac{(\Omega_D)^2 \, [2m]^{D/2}}{h^D D} \; \frac{E^D}{A^{D/2}} \int_0^{\pi/2} \cos^{D+2}\theta \, \sin^{D-1}\theta \, d\theta$$

We now use the relation

$$\int_0^{\pi/2} \sin^{n-1}\theta \, \cos^{n-1}\theta \, d\theta = \frac{1}{2} \, \frac{\Gamma(\frac{n}{2}) \, \Gamma(\frac{m}{2})}{\Gamma(\frac{m+n}{2})}$$

$$\Omega_D = \frac{2 \, \pi^{D/2}}{\Gamma(\frac{D}{2})}$$

From these equations we obtain

$$\text{(II.5.8)} \quad E = \frac{h}{2\pi} \, \omega \, (D! \, N_p)^{1/D} \qquad \text{where} \quad \omega = \sqrt{\frac{k_0 (N_p - 1) k}{m}}$$

but using this result with (II.5.8), and carrying out the indicated integraions of (II.5.6) we obtain the equation

$$\langle H \rangle = \frac{D}{(D+1)!} \, (D! \, N_p)^{\frac{D+1}{D}} \, \hbar \sqrt{\frac{k_0 + (N_p - 1) k}{m}}$$

For the closed shell structure where $N_p = \binom{N+D-1}{D}$ we get the Thomas Fermi approximation

$$\text{(II.5.9)} \quad \langle H \rangle = \frac{D}{(D+1)!} \left[\frac{(N+D-1)!}{(N-1)!}\right] \cdot \left[\frac{(N+D-1)!}{(N-1)!}\right]^{1/D} \hbar \sqrt{\frac{k_0 + (N_p - 1) k}{m}}$$

And for comparison the Hartree-Fock minus the exchange term discussion in Section 4 gives:

$$\langle H\rangle = \frac{D}{(D+1)!}\left[\frac{(N+D-1)!}{(N-1)!}\right]\cdot\left(N+\frac{D-1}{2}\right)\hbar\sqrt{\frac{k_0+(N_p-1)k}{m}} .$$

# Appendix 1

## Part I: Wigner-Moyal (Dirac) Density

Notation:

| | |
|---|---|
| $u$ | scalar quantity |
| $\underset{\sim}{u}$ | vector quantity |
| $\bar{u}$ | operator with one component |
| $\underset{\sim}{\bar{u}}$ | operator with several components |
| $\langle P(\underset{\sim}{\bar{p}},\underset{\sim}{\bar{x}})\rangle$ | expectation value of operator $P(\underset{\sim}{\bar{p}},\underset{\sim}{\bar{x}})$ |

Consider a Moyal ordered operator $P(p,x)$

$$P(\bar{p},\bar{x}) = \sum_{k,\ell} p_{k,m}\{\bar{p}^k,\bar{x}^m\} \tag{A.1.1}$$

where

$$\{\bar{p}^k,\bar{x}^m\} = [1/\binom{k+m}{m}]\cdot\left(\begin{array}{l}\text{sum of all possible orders}\\ \text{of } k\ \bar{p}\text{'s and } m\ \bar{q}\text{'s}\end{array}\right) \tag{A.1.2}$$

If we limit ourselves for the moment to an operator for which a fourier transform exists, we may write:

$$P(\bar{p},\bar{x}) = \iint d\tau\, d\theta\, f(\tau,\theta)\, \exp\,(i\tau\bar{p} + i\theta\bar{x}) \ . \tag{A.1.3}$$

Using the corresponding scalar function

$$P(p,q) = \sum p_{k,m}\, p^k\, q^m \tag{A.1.4}$$

$$(\mathrm{A.1.5}) \quad f(\tau,\theta) = (1/2\pi)^2 \iint dp\, dq\, P(p,q) \exp\,(-i\tau p - i\theta q)$$

so

$$(\mathrm{A.1.6}) \quad P(\bar{p},\bar{x}) = (1/2\pi)^2 \iint d\tau\, d\theta\, dp\, dq\, P(p,q) \cdot$$

$$\cdot \exp\,(i\tau(\bar{p}-p) + i\theta(\bar{x}-q))$$

$$(\mathrm{A.1.7}) \quad P(\bar{p},\bar{x}) = (1/2\pi)^2 \iint dx\, d\tau\, d\theta\, dp\, dq\, P(p,q)\psi^*(x) \cdot$$

$$\cdot \exp\,(i\tau(\bar{p}-p)+i\theta(\bar{x}-q))\psi(x)\ .$$

Here we use the equation:

$$(\mathrm{A.1.8}) \quad e^{i\tau\bar{p}+i\theta\bar{x}} = e^{\frac{i}{2}\tau\bar{p}}\, e^{i\theta\bar{x}}\, e^{\frac{i}{2}\tau\bar{p}}\ ;$$ [9]

$$(\mathrm{A.1.9}) \quad \langle P(\bar{p},\bar{x})\rangle = \frac{1}{(2\pi)^2} \iint dx\, d\tau\, d\theta\, dp\, dq\, P(p,q) \cdot$$

$$\cdot \left(e^{-\frac{i\tau\bar{p}}{2}}\psi^*(x)\right) e^{-i\tau p - i\theta(x-q)} \left(e^{\frac{i\tau\bar{p}}{2}}\psi(x)\right).$$

Noting that $e^{i\tau\bar{p}/2}\psi(x) = e^{(\hbar\tau/2)\partial/\partial x}\psi(x) = \psi(x+\hbar\tau/2)$ and then integrating out $\theta$ and then $q$, we get:

$$(\mathrm{A.1.10}) \quad \langle P(\bar{p},\bar{x})\rangle = \frac{1}{2\pi} \iint dx\, dp\, P(p,x) \int d\tau\, \psi^*(x-\frac{\hbar\tau}{2}) \cdot$$

$$\cdot\, e^{-i\tau p}\, \psi(x+\frac{\hbar\tau}{2}).$$

---

[9] W. O. Kermack and W. H. McCrea, Proc. Edinburgh Math. Soc. Vol. II, Series 2, (1931), p. 224.

From this we see it is natural to consider the phase space distribution function:

$$(A.1.11)\quad \rho(p,x) = \frac{1}{2\pi}\int d\tau\; \psi^{*}(x-\frac{\hbar\tau}{2})\;\psi(x+\frac{\hbar\tau}{2})\; e^{-i\tau p}.$$

This is generally known as the Wigner or Wigner-Moyal density. Of course this may be easily generalized to multiple dimensions, multiple states, and multiple particles.

$$(A.1.12)\quad \rho(\underset{\sim}{p},\underset{\sim}{x}) = \frac{1}{(2\pi)^{D}}\iint d\underset{\sim}{\tau}\; \rho(\underset{\sim}{x}+\frac{\hbar\underset{\sim}{\tau}}{2},\; \underset{\sim}{x}-\frac{\hbar\underset{\sim}{\tau}}{2})\, e^{-i\underset{\sim}{\tau}\cdot\underset{\sim}{p}},$$

where D equals the number of dimensions and the better known Dirac density.[10]

Rewriting (A.1.10), we have

$$(A.1.13)\quad \langle P(\bar{p},\bar{x})\rangle = \iint dp\; dx\; P(p,x)\;\rho(p,x).$$

To generalize this relation for operators with no fourier transform we can use the generating operator:

$$(A.1.14)\quad P(\bar{p},\bar{x}) = \iint d\tau\; d\theta\; e^{i(\tau a\bar{p}+\theta b\bar{x})}\; e^{-\tau^{2}-\theta^{2}}.$$

(The coefficient $a^{k}b^{m}$ will be some constant multiple of $\{\bar{p}^{k},\bar{x}^{m}\}$.

---

[10] L. D. Landau and E. M. Lifshitz, Quantum Mechanics, (Reading, Mass., Addison-Wesley's, 1958), p. 35 ff.

Thus we see equation (A.1.13) will apply to any operator $P(\bar{p},\bar{x})$ of the form $P(\bar{p},\bar{x}) = \sum_{k,m} p_{k,m}\{\bar{p}^k,\bar{x}^m\}$ if $\sum_{k,m} p_{k,m} \langle\{\bar{p}^k,\bar{x}^m\}\rangle$ is convergent.

It is now clear that we may expand this last generalization to multiple dimensions so:

if

$$P(\underset{\sim}{\bar{p}},\underset{\sim}{\bar{x}}) = \sum_{k,m} p_{k,m}\{\underset{\sim}{\bar{p}}^k,\underset{\sim}{\bar{x}}^m\}$$

and

$$\sum_{k,m} p_{k,m} \langle\{\underset{\sim}{\bar{p}}^k,\underset{\sim}{\bar{x}}^m\}\rangle$$

is convergent, then

$$\text{(A.1.15)} \qquad \langle P(\underset{\sim}{\bar{p}},\underset{\sim}{\bar{x}})\rangle = \iint d\underset{\sim}{p}\; d\underset{\sim}{x}\; P(\underset{\sim}{p},\underset{\sim}{x})\, \rho(\underset{\sim}{p},\underset{\sim}{x})$$

where $\rho(\underset{\sim}{p},\underset{\sim}{x})$ is the Wigner-Moyal density defined in equation (A.1.12).

Note! I have used here the same functional notation for the Dirac and Wigner-Moyal densities, but this should not create confusion since the Wigner-Moyal density is a function of both momentum and coordinates, while the Dirac density is a function of coordinates only.

Historically, there is interesting comment to be made. P.A.M. Dirac appears to be actually the first man to use this phase space density referring to it as a "pseudo classical density" [1]. Dirac's "pseudo classical density" was not properly normalized and

Dirac failed to observe that expectation values for measurable quantities could be computed directly without converting back to the Dirac density.

In 1932 E. Wigner published a brief paper specifically on this density without reference to the Dirac paper [10]. He noted that this density is not a genuine probability distribution (it is always real but it can take on negative values). More importantly however he indicated that for many computational purposes this phase space density can be treated as if it were a genuine probability density.

For several years afterwards this phase space density was known as the Wigner density. Then in 1949 J. E. Moyal published an extensive paper on this phase space density [11]. (Most of the arithmetic in the opening paragraphs of this appendix were lifted directly from Moyal's paper.) Since the publication of this paper, this density has generally been referred to in the literature as the Wigner-Moyal density.

One of the things that Moyal observed was that this density satisfies an equation very close to the classical Liouville theorem, namely:

$$\text{(A.1.16)} \quad \frac{\partial}{\partial t} F(p,q,t) = \frac{2}{\hbar} \sin \frac{\hbar}{2} \left[\frac{\partial}{\partial p_F} \frac{\partial}{\partial q_H} - \frac{\partial}{\partial p_H} \frac{\partial}{\partial q_F}\right] \cdot H(p,q)\, F(p,q,t).$$

This is a pretty equation and it gives some indication of how close the Wigner-Moyal density is to the classical density. However as with all such dynamical equations, it is necessary to insert proper boundary conditions. For the corresponding classical equation:

$$\frac{\partial F}{\partial t}(p,q,t) = \frac{\partial H}{\partial p} \cdot \frac{\partial F}{\partial q} - \frac{\partial H}{\partial q} \cdot \frac{\partial F}{\partial p}$$

all non-negative functions $F(p,q,0)$ which are first order differentiable in p and q are physically admissible as initial boundaries. Also any non-negative $F(p,q)=f(H(p,q))$, where f is arbitrary, is physically admissible as a stationary solution.

However in quantum mechanics this is no longer the case. For instance for the harmonic oscillator $f(H(p,q))$ where f is arbitrary is a stationary solution of (A.1.16) but may not correspond to any Wigner-Moyal density.

It is not at all clear what boundary conditions are necessary for (A.1.16) and without them it becomes almost useless.

Despite this drawback several physicists in recent years have found the Wigner-Moyal density useful for some kinds of computations, just as Dirac did back in 1930.

In 1957, Kompaneets and Pavlovskii published a paper showing that the Thomas-Fermi density for the atom with Weisacker and exchange corrections could be extracted from the Hartree-Fock equations [3]. In this paper Kompaneets and Pavlovskii referred to the "pseudo classical density" of Dirac's 1930 paper and then rederived the Moyal bracket equation (A.1.16). From an esthetic point of view there were two shortcomings in their paper. The first shortcoming was that Kompaneets and Pavlovskii were apparently unaware of the work of Wigner or Moyal and so there is no indication of the fact that it is unnecessary to convert back to the Dirac density in order to compute expectation values. The second and perhaps more serious shortcoming resulted from their use of the Moyal bracket equation (A.1.16). They "solved" the equation without introducing the necessary boundary conditions and thus, they were unable to show that their solution was necessarily the right solution.

In 1960, Baraff and Borowitz corrected the second shortcoming by using what amounts to a Wigner-Moyal Green's function [9]. However, Baraff and Borowitz also did not relate their work to that of Wigner and Moyal so their paper also suffered slightly from the first shortcoming in the Kompaneets and Pavlovskii paper.

In closing let us look at the Wigner-Moyal densities for a few simple problems.

For the minimum wave packet:

$$\psi(x) = [2\pi(\Delta x)^2]^{-1/4} \exp\left[ -\frac{(x-\langle x\rangle)^2}{4(\Delta x)^2} + \frac{i\langle p\rangle x}{\hbar} \right] \tag{A.1.17}$$ [11]

---

[11] Schiff, Quantum Mech., p. 57

Using equation (A.1.11) we compute the corresponding Wigner-Moyal density and get:

$$(A.1.18) \qquad \rho(p,x) = \frac{1}{\pi\hbar} \exp \left[ - \frac{(x-\langle x\rangle)^2}{2(\Delta x)^2} - \frac{(p-\langle p\rangle)^2}{2(\Delta p)^2} \right]$$

where

$$(\Delta x)^2 = \langle (x-\langle x\rangle)^2 \rangle$$

$$(\Delta p)^2 = \langle (p-\langle p\rangle)^2 \rangle$$

and

$$(\Delta x)^2(\Delta p)^2 = \frac{\hbar^2}{4} .$$

In the cases of the free particle and the harmonic oscillator, the Moyal brackets reduce to the classical Poisson brackets. Thus for these two cases we should expect some very classical looking solutions. Using equations (A.1.11) and (A.1.12) and following the techniques used by Schiff on pp. 56 to 58 and pp. 67 to 69, we get the time development of the minimum wave packet for the free particle (one dimension)

$$(A.1.19) \qquad \rho(p,x) = \frac{1}{\pi\hbar} \exp \left[ - \frac{(p-\langle p_0\rangle)^2}{2(\Delta p_0)^2} - \frac{(x-\langle x_0\rangle - \frac{pt}{m})^2}{2(\Delta x_0)^2} \right]$$

where

$$\langle p_0 \rangle = \langle p \rangle \Big|_{t=0} , \qquad \langle x_0 \rangle = \langle x \rangle \Big|_{t=0}$$

$$(\Delta p_0)^2 = \langle (p-\langle p\rangle)^2 \rangle \Big|_{t=0} , \quad (\Delta x_0)^2 = \langle (x-\langle x\rangle)^2 \rangle \Big|_{t=0}$$

$$(\Delta p_0)^2(\Delta x_0)^2 = \frac{\hbar^2}{4} ,$$

and for the harmonic oscillator (one dimension)

$$(\text{A.1.20}) \qquad \rho(p,x) = \frac{1}{\pi h} \exp \left[ - \frac{(x-\langle x\rangle)^2}{2(\Delta x)^2} - \frac{(p-\langle p\rangle)^2}{2(\Delta p)^2} \right]$$

where

$$\langle x\rangle = \langle x_0\rangle \cos \omega t + \frac{\langle p_0\rangle}{m\omega} \sin \omega t$$

$$\langle p\rangle = \langle p_0\rangle \cos \omega t - \frac{k\langle x_0\rangle}{\omega} \sin \omega t$$

$$(\Delta x)^2 = \frac{\hbar^2}{2m\omega} \qquad (\Delta p)^2 = \frac{m\omega\hbar}{2}$$

and where $\omega$ is the classical frequency $= \sqrt{k/m}$.

In his textbook, Schiff mentions the fact that in coordinate space the free particle minimum wave packet spreads as time increases.

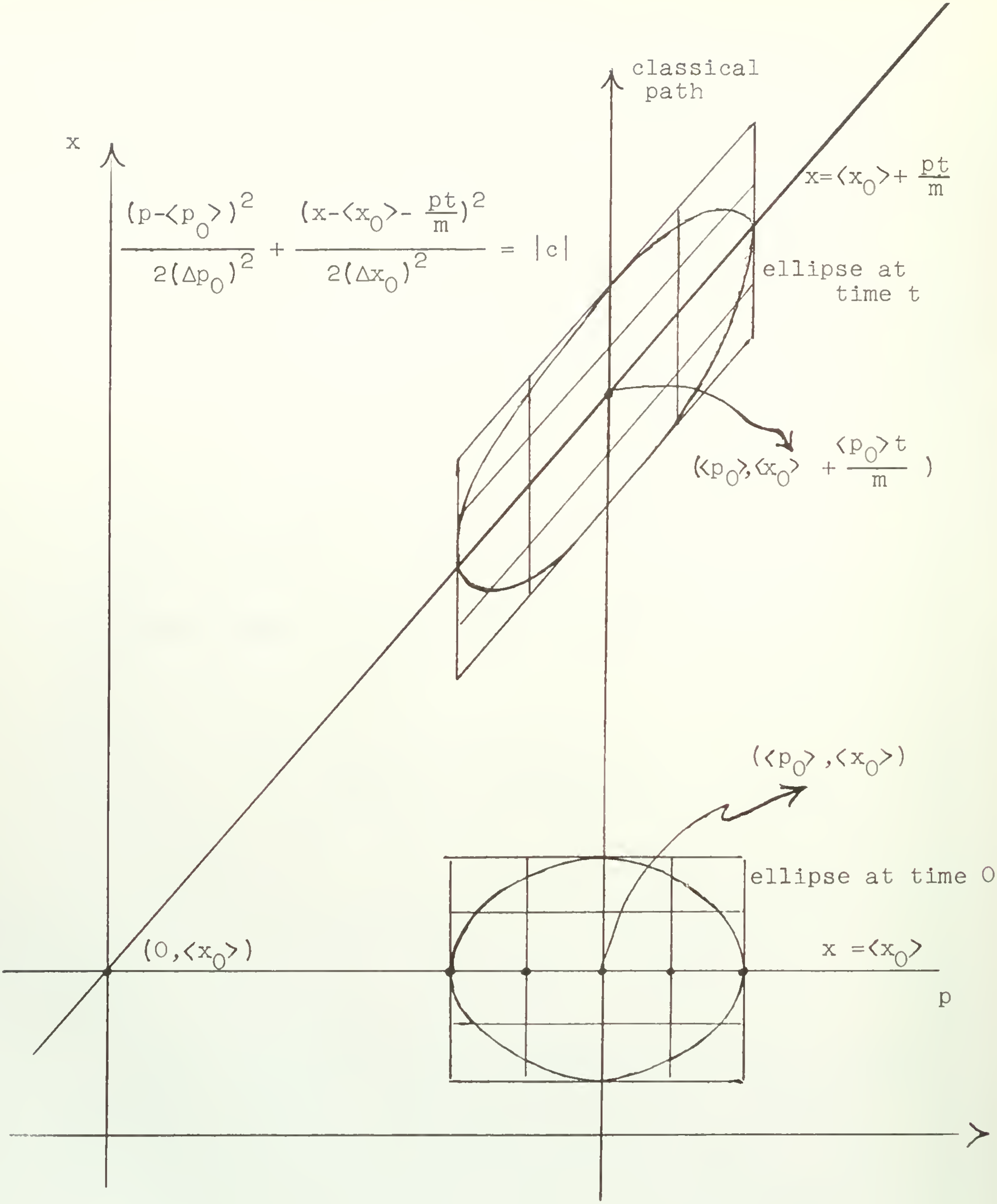
$$(\text{A.1.21}) \qquad \rho(x) = \frac{1}{\sqrt{2\pi\left((\Delta x_0)^2 + \dfrac{(\Delta p_0)^2 t^2}{m^2}\right)}} \cdot \exp \left[ - \frac{\left(x-\langle x_0\rangle - \dfrac{\langle p_0\rangle t}{m}\right)^2}{\left((\Delta x_0)^2 + \dfrac{(\Delta p_0)^2 t^2}{m^2}\right)} \right] .$$

However since the Moyal brackets in this case collapse to Poisson brackets, the Wigner-Moyal density satisfies the conditions of the classical Liouville theorem. Thus as is apparent from the form of (A.1.16), the minimum free particle Wigner-Moyal wave packet moves along the classical path in phase space and it "spreads" only in the sense that it changes shape.

Referring to (A.1.16) and (A.1.19) let us consider the ellipse:

$$\frac{(p-\langle p_0\rangle)^2}{2(\Delta p_0)^2} + \frac{(x-\langle x_0\rangle-\frac{pt}{m})^2}{2(\Delta x_0)^2} = |c|$$

In the figure on the following page, since the area of the little parallelograms remains invariant as t increases, we see by an obvious limiting process that the area of the ellipse remains invariant as t increases.


x
$\frac{(p-\langle p_0\rangle)^2}{2(\Delta p_0)^2} + \frac{(x-\langle x_0\rangle - \frac{pt}{m})^2}{2(\Delta x_0)^2} = |c|$
classical path
$x=\langle x_0\rangle + \frac{pt}{m}$
ellipse at time t
$(\langle p_0\rangle, \langle x_0\rangle + \frac{\langle p_0\rangle t}{m})$
$(\langle p_0\rangle, \langle x_0\rangle)$
ellipse at time 0
$(0, \langle x_0\rangle)$
$x = \langle x_0\rangle$
p

Part II: Kirkwood Density [12].

The arithmetic for the Kirkwood density is much the same as that for the Wigner-Moyal density. The chief difference is that for Kirkwood computations one begins with a "normally" ordered operator.

$$P(\bar{p},\bar{x}) = \sum_{k,m} p_{k,m}\, \bar{x}^k\, \bar{p}^m \quad . \tag{A.1.22}$$

Assuming for the moment that P(p,x) has a Fourier transform we may write

$$P(\bar{p},\bar{x}) = \iint d\tau\, d\theta\, f(\tau,\theta)\, e^{i\theta\bar{x}}\, e^{i\tau\bar{p}} \quad . \tag{A.1.23}$$

Now using the corresponding scalar function

$$P(p,q) = \sum p_{k,m}\, q^k\, p^m$$

we get:

$$P(p,q) = \iint d\tau\, d\theta\, f(\tau,\theta)\, e^{i\theta q}\, e^{i\tau p} \tag{A.1.24}$$

$$f(\tau,\theta) = \frac{1}{(2\pi)^2} \iint P(p,q)\, e^{-i\tau p - i\theta q}\, dp\, dq \tag{A.1.25}$$

$$P(\bar{p},\bar{x}) = \frac{1}{(2\pi)^2} \iint d\tau\, d\theta\, dp\, dq\, e^{i\theta(\bar{x}-q)} \cdot e^{i\tau(\bar{p}-p)}\, P(p,q) \tag{A.1.26}$$

$$\langle P(\bar{p},\bar{x})\rangle = \frac{1}{(2\pi)^2} \iint d\tau \; d\theta \; dp \; dq \; dx \cdot P(p,q) \, \psi^*(x) \, e^{i\theta(\bar{x}-q)} \, e^{i\tau(\bar{p}-p)} \, \psi(x) \tag{A.1.27}$$

$$\langle P(\bar{p},\bar{x})\rangle = \frac{1}{(2\pi)^2} \iint d\tau \; d\theta \; dp \; dq \; dx \cdot P(p,q) \, \psi^*(x) \, e^{i\theta(x-q)} \, \psi(x+\hbar\tau). \tag{A.1.28}$$

Integrating out $\theta$ and then q we get:

$$\langle P(\bar{p},\bar{x})\rangle = \frac{1}{2\pi} \iint dp \; dx \; P(p,x) \cdot \int d\tau \; \psi^*(x) \, e^{-i\tau p} \, \psi(x+h\tau). \tag{A.1.29}$$

We thus define the Kirkwood density $\rho_k(p,q)$

$$\rho_k(p,x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \psi^*(x) \, e^{-i\tau p} \, \psi(x+\hbar\tau) \; d\tau \; . \tag{A.1.30}$$

Then from (A.1.29) and (A.1.30)

$$\langle P(\bar{p},\bar{x})\rangle = \iint dp \; dx \; P(p,x) \; \rho_k(p,x) \tag{A.1.31}$$

In the same fashion as we did for the Wigner-Moyal density, it is possible to extend equation (A.1.31) to apply to operators for which no Fourier transform exist.

And as we did for the Wigner-Moyal density, we may generalize the Kirkwood density to multiple dimensions, multiple particles, and multiple states.

Last we should note two equations used in the main body of the paper (A.1.34) and (A.1.38).

First taking the Fourier inverse of (A.1.30) we get:

$$\text{(A.1.32)} \qquad \int_{-\infty}^{\infty} \rho_k(p,x)\, e^{i\tau' p}\, dp = \psi^*(x)\, \psi(x+\hbar\tau')$$

Substituting $x' = x+\hbar\tau'$ we have:

$$\text{(A.1.33)} \qquad \psi^*(x)\, \psi(x') = \int_{-\infty}^{\infty} \rho_k(p,x)\, e^{i\frac{p(x'-x)}{\hbar}}\, dp$$

Taking complex conjugate of both sides

$$\text{(A.1.34)} \qquad \psi(x)\psi^*(x') = \int_{-\infty}^{\infty} \rho_k^*(p,x)\, e^{i\frac{p(x-x')}{\hbar}}\, dp.$$

Second, to get the operator which transforms the Kirkwood density into the Wigner-Moyal density

$$\text{(A.1.35)} \qquad e^{\frac{-i\hbar}{2}\frac{\partial^2}{\partial p \partial x}} \rho_k(p,x) = \frac{e^{\frac{-i\hbar}{2}\frac{\partial^2}{\partial p\partial x}}}{2\pi} \int_{-\infty}^{\infty} d\tau \cdot e^{-i\tau p}\, \psi^*(x)\, \psi(x+\hbar\tau)$$

$$(A.1.36) \quad e^{-\frac{i\hbar}{2}\frac{\partial^2}{\partial p\partial x}} \rho_k(p,x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\tau \; e^{-i\tau(p-\frac{i\hbar}{2}\frac{\partial}{\partial x})}$$

$$\cdot \; \psi^*(x)\;\psi(x+\hbar\tau)$$

$$(A.1.37) \quad e^{-\frac{i\hbar}{2}\frac{\partial^2}{\partial p\partial x}} \rho_k(p,x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau \; e^{-i\tau p} \; \psi^*(x-\frac{\hbar\tau}{2})\psi(x+\frac{\hbar\tau}{2})$$

Thus

$$(A.1.38) \qquad e^{-\frac{i\hbar}{2}\frac{\partial^2}{\partial p\partial x}} \rho_k(p,x) \;=\; \rho(p,x)$$

# Appendix 2

Here we have essentially copied from the paper by W. Macke and P. Rennert [6].

Consider the operator

$$(A.2.1) \qquad F(u) = e^{-uA} B e^{uA}$$

where A and B are operators and u is a scalar.

$$(A.2.2) \qquad \begin{aligned} F(0) &= B \\ F(1) &= e^{-A} B e^{A} = \sum_{n=0}^{\infty} \frac{F^{(n)}(0)}{n!} \end{aligned}$$

Now

$$F'(u) = -Ae^{-uA} Be^{uA} + e^{-uA} Be^{uA} A = [F(u),A]$$

$$(A.2.3) \qquad F''(u) = [F'(u),A] = [[F(u),A],A]$$

$$F^{(3)}(u) = [[[F(u),A],A],A]$$

$$(A.2.4) \qquad F^{(n)}(0) = [[[\ldots[[F(u),\overset{[1}{A}], \overset{2}{A}] \ldots \overset{n]}{A}] = ([\ ,A])^{n} B$$

From (A.2.2) and (A.2.4) we get

$$(A.2.5) \qquad e^{-A} B e^{A} = e^{([\ ,A])} B$$

Now consider the operator

$$(A.2.6) \qquad \begin{aligned} G(u) &= e^{-uA}\, e^{u(A+B)} \\ G(0) &= 1 \end{aligned}$$

$$(A.2.7) \qquad \begin{aligned} G'(u) &= -\,Ae^{-uA}\, e^{u(A+B)} + e^{-uA}\,(A+B)\, e^{u(A+B)} \\ G'(u) &= e^{-uA}\, B\, e^{u(A+B)} = (e^{u([\ ,A])}\, B)\, G(u). \end{aligned}$$

One should observe that the operators of the form $e^{u([\ ,A])}B$ for different values of u do not commute with one another.

To continue:

$$(A.2.8) \qquad G(u + du) = (1 + du\, e^{u([\ ,A])}\, B)\, G(u)\ .$$

So:

$$(A.2.9) \qquad G(u) = {}^{u}\prod{}^{0}\ e^{du\, e^{u([\ ,A])}B}$$

For our purposes, we make the approximation that $[[[B,A],A],A] \approx 0$.

Then we get

$$(A.2.10) \qquad e^{u([\ ,A])}B \approx B + u[B,A] + \frac{u^2}{2}\,[[B,A],A].$$

Now if we also make the approximation that $B$, $[B,A]$, and $[[B,A],A]$ commute with one another, then the continuous product of (A.2.9) may be rewritten:

$$G(u) \approx e^{\int_0^u (B+u[B,A]+\frac{u^2}{2}[[B,A],A])\,du}$$

(A.2.11)

$$G(u) \approx e^{(uB + \frac{u^2}{2}[B,A] + \frac{u^3}{6}[[B,A],A])}.$$

From (A.2.6) and (A.2.11) setting u = 1, we get

$$e^{(A+B)} \approx e^{A} e^{(B + \frac{1}{2}[B,A] + \frac{1}{6}[[B,A],A])} \tag{A.2.12}$$

## Appendix 3

$$(A.3.1) \qquad A_i(x) = \frac{1}{2\pi} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \exp\left( \frac{it^3}{3} + ixt \right) dt$$

$$(A.3.2) \quad A_i(x)A_i(y) = \frac{1}{4\pi^2} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} dt\ ds$$

$$\cdot \exp\left(\frac{it^3}{3} + \frac{is^3}{3} + ixt + iyt\right)$$

Substitute

$$R = \frac{x+y}{2} \qquad u = t+s \qquad t = \frac{u}{2} + v$$

$$r = x-y \qquad v = \frac{t-s}{2} \qquad s = \frac{u}{2} - v$$

Then:

$$(A.3.3) \quad A_i(R+\tfrac{r}{2})A_i(R-\tfrac{r}{2}) = \frac{1}{4\pi^2} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} du \exp\left( \frac{iu^3}{12} + iRu \right)$$

$$\cdot \int_{-\infty}^{\infty} dv \exp\left(iuv^2 + irv\right)$$

$$(A.3.4)\quad \frac{d^{2m}}{dr^{2m}} A_i(R+\frac{r}{2})A_i(R-\frac{r}{2})\Big|_{r=0} = \frac{(-1)^m}{4\pi^2} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} du$$

$$\cdot \exp\left(\frac{iu^3}{12} + iRu\right) \int_{-\infty}^{\infty} v^{2m} \exp iuv^2 \, dv$$

but

$$(A.3.5)\quad \int_{-\infty}^{\infty} dv \; v^{2m} \exp iuv^2 = 2 \int_{-\infty}^{\infty} dv \; v^{2m} \exp iuv^2$$

Let $\omega = e^{-i\pi/2} uv^2$ and then

$$(A.3.6)\quad \int_{-\infty}^{\infty} dv \; v^{2m} \exp iuv^2 = \frac{(e^{\frac{i\pi}{2}})^{m+\frac{1}{2}}}{u^{m+1/2}} \int_0^{\infty} \omega^{m-1/2} e^{-\omega} d\omega$$

$$(A.3.7)\quad \int_{-\infty}^{\infty} dv \; v^{2m} \exp iuv^2 = \frac{(e^{\frac{i\pi}{2}})^{m+\frac{1}{2}}}{u^{m+1/2}} \Gamma(m+\frac{1}{2}) .$$

Thus

$$(A.3.8)\quad \frac{d^{2m}}{dr^{2m}} A_i(R+\frac{r}{2})A\,(R-\frac{r}{2})\Big|_{r=0} = \frac{(-1)^m e^{\frac{i\pi}{2}(m+\frac{1}{2})} \Gamma(m+\frac{1}{2})}{4\pi^2}$$

$$\cdot \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \frac{du \; \exp(\frac{iu^3}{12} + iRu)}{u^{m+1/2}} .$$

Let $u = a\omega$;

$$(A.3.9)\quad \frac{d^{2m}}{dr^{2m}} A_i(R+\frac{r}{2})\; A(R-\frac{r}{2})\Bigg|_{r=0}$$

$$= \frac{(-1)^m e^{\frac{i\pi}{2}(m+\frac{1}{2})}\,\Gamma(m+\frac{1}{2})}{4\pi^2\; a^{m-1/2}} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \frac{du\;\exp(\frac{ia^3u^3}{12}+iRau)}{u^{m+1/2}}$$

To get a closed from for (I.5.17) and (I.5.18) of the main text when D is an odd integer we set:

$$(A.3.10)\quad a^3 = \frac{\hbar^2|\underset{\sim}{\nabla}V|^2}{2m}, \qquad aR = -\,[E - V(\underset{\sim}{r})]$$

$$\text{or}\qquad R = \frac{-\,\alpha}{4^{1/3}} \quad \text{where} \quad \alpha = \frac{2m[E - V(\underset{\sim}{r})]}{(m\hbar\,\underset{\sim}{\nabla}V)^{2/3}}$$

then

$$(A.3.11)\quad \frac{e^{\frac{i\pi}{2}(m-\frac{1}{2})}}{2\pi i} \int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon} \frac{d\omega}{\omega^{m+1/2}}\, e^{-i\omega(E-V(\underset{\sim}{r}))+\frac{i\omega^3\hbar^2}{24m}|\underset{\sim}{\nabla}V|^2}$$

$$= \frac{(-1)^{m+1}2\pi(2mh|\underset{\sim}{\nabla}V|)^{\frac{2m-1}{3}}}{(2m)^{\frac{2m-1}{2}}\quad \Gamma(m+\frac{1}{2})} \;\frac{d^{2m}}{dr^{2m}} A_i(\frac{-\alpha}{4^{1/3}}+\frac{r}{2})A_i(\frac{-\alpha}{4^{1/3}}-\frac{r}{2})\Bigg|_{r=0}$$

Thus using (I.5.17) of the main text we let $m = \frac{D+1}{2}$ and get

$$(A.3.12)\quad \rho(\underset{\sim}{r}) = \frac{(-1)^{\frac{D+1}{2}}\,4\pi\,\Omega_D(2m\hbar|\underset{\sim}{\nabla}V|)^{D/3}}{D\;h^D}\;\frac{d^{D+1}}{du^{D+1}}$$

$$\cdot\; A_i(\frac{-\alpha}{4^{1/3}}+\frac{u}{2})\; A_i(\frac{-\alpha}{4^{1/3}}-\frac{u}{2})\Bigg|_{u=0},$$

$$D = 1,3,5,\;\ldots\;.$$

And using (I.5.18) of the main text we let $m = \frac{D+3}{2}$ and get:

$$(\text{A.3.13}) \quad t(\underset{\sim}{r}) = \frac{(-1)^{\frac{D+3}{2}} 4\pi\, \Omega_D (2mh|\underset{\sim}{\nabla} V|)^{\frac{D+2}{3}}}{(D+2)\ 2m\ h^D} \frac{d^{D+3}}{du^{D+3}}$$

$$\cdot\ A_i\left(\frac{-\alpha}{4^{1/3}} + \frac{u}{2}\right) A_i\left(\frac{-\alpha}{4^{1/3}} - \frac{u}{2}\right)\Bigg|_{u=0},$$

$$D = 1,3,5,\ \ldots\ .$$

While we are at it we notice that by comparing (I.5.28) of the main text with (A.3.12) we see that:

$$(\text{A.3.14}) \quad \int_{-\infty}^{\alpha} (\alpha - t)^{\frac{2k-1}{2}} A_i(-t)\, dt$$

$$= (-1)^k\, 2\pi\, 2^{\frac{2k-1}{3}} \frac{d^{2k}}{du^{2k}} \left[A_i\left(\frac{-\alpha}{4^{1/3}} + \frac{u}{2}\right) A_i\left(\frac{-\alpha}{4^{1/3}} - \frac{u}{2}\right)\right]\Bigg|_{u=0}$$

$$\text{for } k = 0,1,2,\ldots\ .$$

# Appendix 4

Asymptotic Expansions of the mass density $\rho(\underset{\sim}{r})$ and kinetic energy density $t(\underset{\sim}{r})$.

From the main text let us rewrite equations (I.5.17) and (I.5.18)

$$\text{(I.5.17)}\quad \rho(r) = -\frac{\Omega_D}{h^D}(2m)^{D/2}\,\Gamma\left(\frac{D}{2}\right)\frac{e^{\frac{i\pi D}{4}}}{2\pi i}\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon}\frac{d\omega}{\omega^{\frac{D+2}{2}}}$$

$$\cdot\; e^{-i\omega(E-V(\underset{\sim}{r}))+\frac{i\omega^3h^2}{24m}|\underset{\sim}{\nabla}V|^2}$$

$$\text{(I.5.18)}\quad t(\underset{\sim}{r}) = -\frac{\Omega_D}{h^D}(2m)^{\frac{D+2}{2}}\,\Gamma\left(\frac{D+2}{2}\right)\frac{e^{\frac{i\pi(D+2)}{4}}}{2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{d\omega}{\omega^{\frac{D+4}{2}}}$$

$$\cdot\; e^{-i\omega(E-V(\underset{\sim}{r}))+\frac{i\omega^3h^2}{24m}|\underset{\sim}{\nabla}V|^2}$$

CASE I (Oscillatory Region $E > V(\underset{\sim}{r})$):

Here we substitute

$$\frac{u^3\beta}{3} = \frac{\omega^3h^2}{24m}|\underset{\sim}{\nabla}V|^2$$

$$u\beta = \omega(E-V(\underset{\sim}{r}))$$

and get

$$\text{(A.4.1)}\quad \rho(\underset{\sim}{r}) = -\frac{\Gamma(D/2)\Omega_D}{h^D}\left[\frac{2m(E-V(\underset{\sim}{r}))}{\beta}\right]^{D/2}\frac{e^{\frac{i\pi D}{4}}}{2\pi i}$$

$$\cdot\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{du}{u^{\frac{D+2}{2}}}\exp\left[i\beta\left(\frac{u^3}{3}-u\right)\right]$$

$$(A.4.2) \quad t(\underset{\sim}{r}) = - \frac{\Gamma(\frac{D+2}{2})\Omega_D}{2m\ h^D} \left[ \frac{2m(E-V(\underset{\sim}{r}))}{\beta} \right]^{\frac{D+2}{2}} \frac{e^{\frac{i\pi(D+2)}{4}}}{2\pi i} \cdot \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \frac{du}{u^{\frac{D+4}{2}}} \exp\left[i\beta\left(\frac{u^3}{3} - u\right)\right]$$

where

$$(A.4.3) \qquad \beta = \frac{[2m(E - V(\underset{\sim}{r}))]^{3/2}}{mh\ |\underset{\sim}{\nabla} V|}$$

It is clear that to find the asymptotic expansions for (A.4.1) and (A.4.2) we need only consider:

$$(A.4.4) \qquad J_D = - \frac{e^{\frac{i\pi D}{4}}}{2\pi i} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \frac{du}{u^{\frac{D+2}{2}}} \exp\left[i\beta\left(\frac{u^3}{3} - u\right)\right] .$$

To get the path of steepest descent, let

$$h(u) = i\left(\frac{u^3}{3} - u\right)$$

$$h'(u) = i(u^2 - 1)$$

So we get the saddle points $u = \pm 1$.

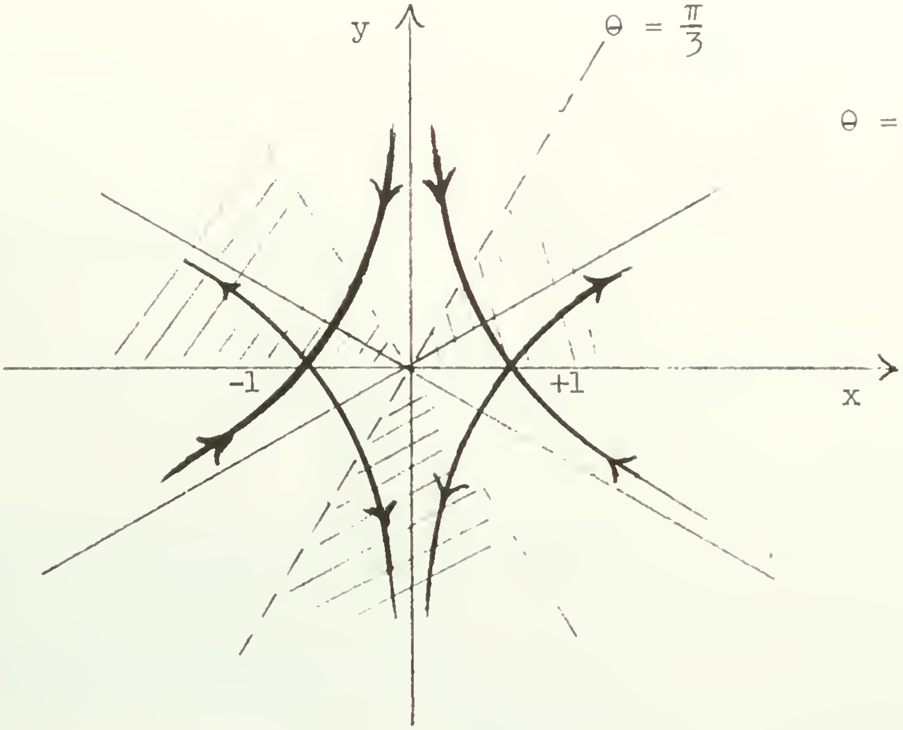
Letting $u = x + iy$ we find that the equation $I_m(h(u))=I_m(h(1))$ corresponds to the equation:

$$y^2 = \frac{(x-1)^2(x+2)}{3x}$$

and the equation $I_m(h(u)) = I_m(h(-1))$ corresponds to the equation:

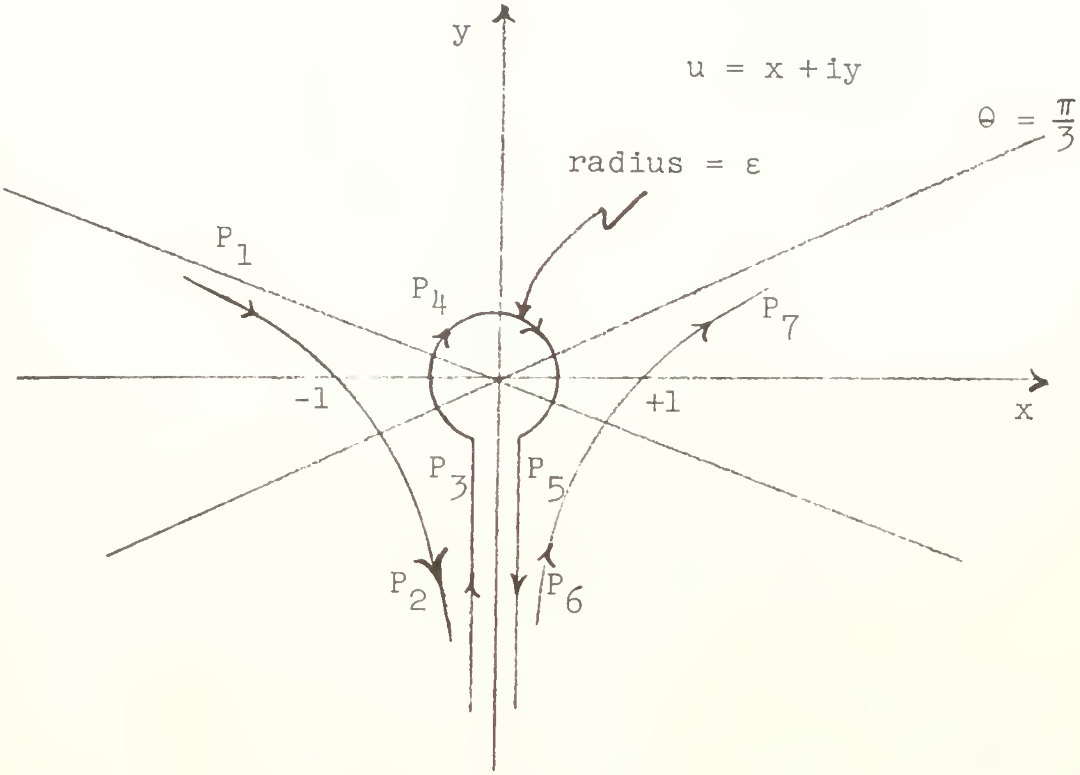
$$y^2 = \frac{(x+1)^2(x-2)}{3x} .$$

We thus get the following graph for lines of steepest descent:



Here the arrows point in the direction of steepest descent.

Thus we choose for the path of integration:



We now designate the contribution to $J_D$ from the path segment $P_k$ as $J_D^k$.

Now $J_D^1$, $J_D^2$, $J_D^6$ and $J_D^7$ may be evaluated by standard methods [13].

Carrying out the computations, the author got the following answer.

$$
\begin{aligned}
J_D^1 + J_D^2 + J_D^6 + J_D^7 \sim \\
& - \frac{\sin\left(\frac{2\beta}{3} + \frac{\pi(3-D)}{4}\right)}{\pi} \left[ \sum_{n=0}^{\infty} \frac{(-1)^n\, \Gamma(6n + \frac{1}{2})}{(4n)!\; 3^{4n}\; \beta^{2n+1/2}} \right. \\
& \left. - \frac{1}{\Gamma(\frac{D+2}{2})} \sum_{n=0}^{\infty} \frac{(-1)^n\, \Gamma(2n+ \frac{5}{2})\, A^D_{4n+3}}{\beta^{2n+ 5/2}} \right] \\
& + \frac{\cos\left(\frac{2\beta}{3} + \frac{\pi(3-D)}{4}\right)}{\pi} \left[ \sum_{n=0}^{\infty} \frac{(-1)^n\, \Gamma(6n + \frac{7}{2})}{(4n+2)!\; 3^{4n+2}\; \beta^{2n+ 3/2}} \right. \\
& \left. + \frac{1}{\Gamma(\frac{D+2}{2})} \sum_{n=0}^{\infty} \frac{(-1)^n\, \Gamma(2n+ \frac{3}{2})\, A^D_{4n+1}}{\beta^{2n+ 3/2}} \right]
\end{aligned}
\tag{A.4.5}
$$

where

$$
\begin{aligned}
A_n^D = \sum_{k=0}^{n} & \frac{\Gamma(\frac{3n-3k+1}{2})}{3^{n-k}(n-k)!\; \Gamma(\frac{n-k+1}{2})(k+1)!} \\
& \cdot \sum_{\ell=0}^{k} \frac{\Gamma(k-\ell+ \frac{D}{2} +2)\; \Gamma(\ell+ \frac{k}{2} + \frac{1}{2})}{3^{\ell}\; \Gamma(\frac{k+1}{2})} \binom{k}{\ell} .
\end{aligned}
$$

For $J_D^3$, $J_D^4$, $J_D^5$ set $\varepsilon = 1/\beta$.

For $J_D^3$, let $u = e^{3\pi i/2}\varepsilon\omega = e^{3\pi i/2}\frac{\omega}{\beta}$ and

for $J_D^5$, let $u = e^{-i\pi/2}\,\varepsilon\omega = e^{-i\pi/2}\frac{\omega}{\beta}$ . Then we get

$$\text{(A.4.6)}\quad J_D^3 + J_D^5 = -\frac{\beta^{D/2}\sin\frac{\pi D}{2}}{\pi}\int_1^{\infty}\frac{e^{-\omega}\, e^{-\frac{\omega^3}{3\beta^2}}}{\omega^{\frac{D+2}{2}}} .$$

For $J_D^4$ let $u = \varepsilon e^{i\theta} = \frac{1}{\beta} e^{i\theta}$

$$\text{(A.4.7)}\quad J_D^4 = \frac{\beta^{D/2} e^{\frac{i\pi D}{4}}}{2\pi}\int_{-\pi/2}^{3\pi/2} d\theta\, e^{-\frac{i\theta D}{2}}\, e^{-ie^{i\theta}}\, e^{\frac{i\, e^{i3\theta}}{3\beta^2}} .$$

When D is even, $J_D^3 + J_D^5 = 0$ and

$$\text{(A.4.8)}\quad J_D^4 = \frac{\beta^{D/2} e^{\frac{i\pi D}{4}}}{2\pi}\int_{-\pi/2}^{3\pi/2} e^{-\frac{i\theta D}{2}} \left(\sum_{k=0}^{\infty}\frac{(-i)^k}{k!}\, e^{ik\theta}\right)$$

$$\cdot\left(\sum_{\ell=0}^{\infty}\frac{(i)^\ell}{\ell!(3\beta^2)^\ell}\, e^{i3\ell\theta}\right)$$

and thus for D even noting that the only terms that contribute to $J_D^4$ are those for which $k = D/2 - 3\ell$, we get

$$\text{(A.4.9)}\quad J_D^3 + J_D^5 + J_D^4 = \beta^{D/2}\sum_{\ell=0}^{[D/6]}\frac{1}{(\frac{D}{2}-3\ell)!\,\ell!\,(3\beta^2)^\ell}\quad \text{(D even)}$$

For D odd things become somewhat more complicated. From (A.4.7) we get

$$\text{(A.4.10)}\quad J_D^4 \sim -\frac{2\beta^{D/2}\sin\frac{\pi D}{2}}{\pi}\sum_{\ell=0}^{\infty}\frac{(-1)^\ell}{\ell!(3\beta^2)^\ell}$$

$$\cdot\sum_{k=0}^{\infty}\frac{(-1)^k}{k![6\ell+2k-D]} .$$

To compute $J_D^3 + J_D^5$ let us substitute $w = u^2$ and we get

$$(A.4.11)\quad J_D^3 + J_D^5 = \frac{2\beta^{D/2} \sin \frac{\pi D}{2}}{\pi} \int_1^{\infty} u^{-(D+1)} e^{-u^2} \cdot \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell}\, u^{6\ell}}{\ell!\,(3\beta^2)^{\ell}} .$$

Now if we make use of the equation

$$(A.4.12)\quad \int_x^{\infty} e^{-t^2}\, dt = \frac{\sqrt{\pi}}{2} - e^{-x^2} \sum_{n=0}^{\infty} \frac{2^k\, x^{2k+1}}{1\cdot 3\cdot \cdots (2k+1)} ,$$ [12]

it is possible to show that

$$(A.4.13)\quad \int_x^{\infty} t^{2N} e^{-t^2}\, dt = \frac{\Gamma(N+\frac{1}{2})}{2} - e^{-x^2} \sum_{k=0}^{\infty} \frac{2^k\, x^{2N+1+2k}}{(2N+1)(2N+3)\ldots(2N+1+2k)}$$

thus

$$(A.4.14)\quad J_D^3 + J_D^5 \sim \frac{\beta^{D/2} \sin \frac{\pi D}{2}}{\pi} \cdot \left[ \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell}}{\ell!(3\beta^2)^{\ell}} (\Gamma(3\ell - \frac{D}{2}) - 2e^{-1} \sum_{k=0}^{\infty} \frac{2^k}{(6\ell-D)(6\ell-D+2)\ldots(6\ell-D+2k)}) \right]$$

---

[12] Handbook of Math. Functions, edited by Milton Abramowitz and Irene A. Stegun (New York, Dover Publications, Inc. 1965), p. 297 (7.1.6).

On the other hand one can show by multiplication of series that:

$$(\text{A.4.15})\quad e^{x^2}\sum_{k=0}^{\infty}\frac{(-1)^k\,x^{2k-D+6\ell}}{k!(2k-D+6\ell)}$$

$$=\sum_{k=0}^{\infty}x^{2k-D+6\ell}\sum_{n=0}^{k}\frac{(-1)^n}{(k-n)!n!(2k-D+6\ell)}\,.$$

And by induction on k we have:

$$(\text{A.4.16})\quad \sum_{n=0}^{k}\frac{(-1)^n}{(k-n)!n!(2k-D+6\ell)}=\frac{2^k}{(6\ell-D)(6\ell-D+2)\ldots(6\ell-D+2k)}$$

Setting $x = 1$ it is now clear that:

$$(\text{A.4.17})\quad e^{-1}\sum_{k=0}^{\infty}\frac{2^k}{(6\ell-D)(6\ell-D+2)\ldots(6\ell-D+2k)}=$$

$$=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!(6\ell+2k-D)}$$

Now using (A.4.17) to add (A.4.10) and (A.4.14) we arrive at the expansion:

$$(\text{A.4.18})\quad J_D^3+J_D^5+J_D^4\sim\frac{\beta^{D/2}\sin\frac{\pi D}{2}}{\pi}\sum_{\ell=0}^{\infty}\frac{(-1)^\ell}{\ell!(3\beta^2)^\ell}\,\Gamma(3\ell-\tfrac{D}{2}),$$

(D odd).

Finally using the relation

$$\Gamma(3\ell - \tfrac{D}{2}) = \frac{\pi}{\Gamma(\frac{D}{2} - 3\ell + 1)} \cdot \frac{1}{\sin\,(3\ell - \frac{D}{2})\pi} ,$$ [13]

we now see it is possible to combine (A.4.9) and (A.4.18) and arrive at:

$$\text{(A.4.19)} \quad J_D^3 + J_D^5 + J_D^4 \sim \beta^{D/2} \sum_{\ell=0}^{\infty} \frac{1}{\Gamma(\frac{D}{2} - 3\ell + 1)\,\ell!\,(3\beta^2)^{\ell}} ,$$

(D an arbitrary integer).

Thus from (A.4.5) and (A.4.19):

$$\text{(A.4.20)} \quad J_D \sim \beta^{D/2} \sum_{n=0}^{\infty} \frac{1}{\Gamma(\frac{D}{2} - 3n + 1)\,n!\,(3\beta^2)^n}$$

$$\frac{-\sin(\frac{2\beta}{3} + \frac{\pi(3-D)}{4})}{\pi} \left[ \sum_{n=0}^{\infty} \frac{(-1)^n \Gamma(6n + \frac{1}{2})}{(4n)!\,3^{4n} \beta^{2n+1/2}} - \frac{1}{\Gamma(\frac{D+2}{2})} \sum_{n=0}^{\infty} \frac{(-1)^n \Gamma(2n + \frac{5}{2}) A^D_{4n+3}}{\beta^{2n+5/2}} \right]$$

$$+\frac{\cos(\frac{2\beta}{3} + \frac{\pi(3-D)}{4})}{\pi} \left[ \frac{(-1)^n \Gamma(6n + \frac{7}{2})}{(4n+2)!\,3^{4n+2} \beta^{2n+3/2}} + \frac{1}{\Gamma(\frac{D+2}{2})} \sum_{n=0}^{\infty} \frac{(-1)^n \Gamma(2n + \frac{3}{2}) A^D_{4n+1}}{\beta^{2n+3/2}} \right]$$

where

$$A^D_n = \sum_{k=0}^{n} \frac{\Gamma(\frac{3n-3k+1}{2})}{3^{n-k}(n-k)!\,\Gamma(\frac{n-k+1}{2})\,(k+1)!} \sum_{\ell=0}^{k} \frac{\Gamma(k - \ell + \frac{D}{2} + 2)\,\Gamma(\ell + \frac{k}{2} + \frac{1}{2})}{3^{\ell}\;\Gamma(\frac{k+1}{2})} \binom{k}{\ell}$$

and

$$\beta = \frac{[2m|E-V(r))]^{3/2}}{m\hbar\,|\underset{\sim}{\nabla}V|}$$

---

[13] Ibid., p. 256 (6.1.17).

From (A.4.1) and (A.4.4):

$$(A.4.21) \qquad \rho(\underset{\sim}{r}) = \frac{\Gamma(\frac{D}{2})\Omega_D}{h^D}\left[\frac{2m(E-V(\underset{\sim}{r}))}{\beta}\right]^{D/2} J_D \qquad (E > V(\underset{\sim}{r}))$$

and from (A.4.2) and (A.4.4) we get

$$(A.4.22) \qquad t(\underset{\sim}{r}) = \frac{\Gamma(\frac{D+2}{2})\Omega_D}{2m\ h^D}\left[\frac{2m(E-V(\underset{\sim}{r}))}{\beta}\right]^{\frac{D+2}{2}} J_{D+2}$$

Case II (Exponentially Decreasing Region E < V($\underset{\sim}{r}$)):

Here we modify (I.5.17) and (I.5.18) of the main text by substituting:

$$\frac{u^3\beta'}{3} = \frac{\omega^3\hbar^2|\underset{\sim}{\nabla}V|^2}{24\ m}$$

$$u\beta' = \omega(V - E)$$

thus:

$$(A.4.23)\ \rho(\underset{\sim}{r}) = \frac{-\Gamma(\frac{D}{2})\,\Omega_D}{h^D}\left[\frac{2m(V(\underset{\sim}{r})-E)}{\beta'}\right]^{D/2}$$

$$\cdot\ \frac{e^{\frac{i\pi D}{4}}}{2\pi i}\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}\frac{du}{u^{\frac{D+2}{2}}}\ \exp i\beta'(\frac{u^3}{3} + u)$$

and

$$(A.4.24) \quad t(\underset{\sim}{r}) = - \frac{\Gamma(\frac{D+2}{2})\,\Omega_D}{2m\ h^D} \left[ \frac{2m(V(\underset{\sim}{r})-E)}{\beta'} \right]^{\frac{D+2}{2}}$$

$$\cdot \frac{(e^{i\pi})^{\frac{D+2}{4}}}{2\pi i} \int_{-\infty + i\varepsilon}^{+\infty + i\varepsilon} \frac{du}{u^{\frac{D+4}{2}}} \exp\ (i\beta'(\frac{u^3}{3} + u))$$

where

$$\beta' = \frac{[2m(V(r)-E)]^{3/2}}{m\hbar\ |\underset{\sim}{\nabla} V|}$$

Here we proceed similarly to Case I and consider only the integral

$$(A.4.25) \quad I_D = - \frac{e^{\frac{i\pi D}{4}}}{2\pi i} \int_{-\infty + i\varepsilon}^{+\infty + i\varepsilon} \frac{du}{u^{\frac{D+2}{2}}} \exp\ i\beta'(\frac{u^3}{3} + u)$$

Now

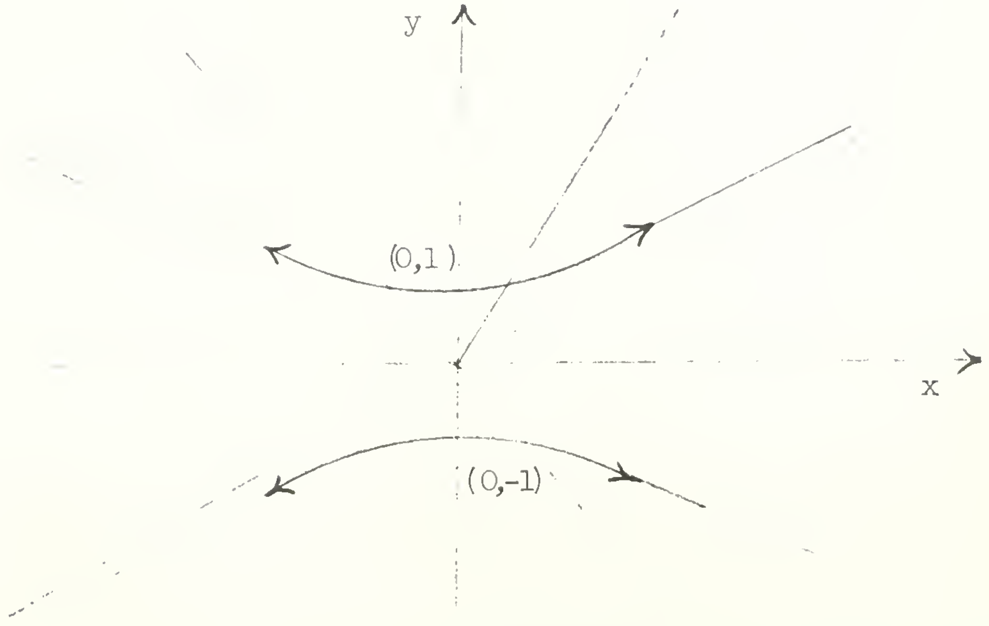
$$h(u) = i(\frac{u^3}{3} + u)$$

$$h'(u) = i(u^2 + 1)\ .$$

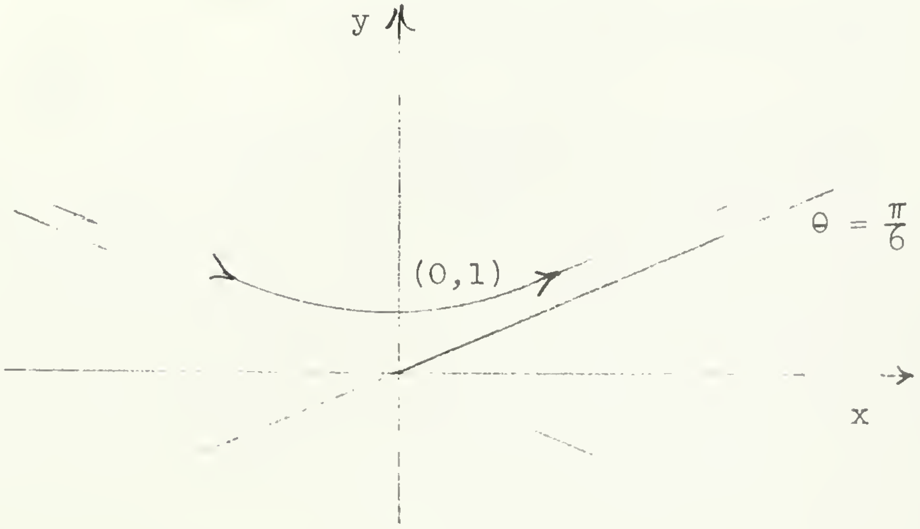
So we get the saddle points $u = \pm\, i$. Letting $u = x + iy$ we find that $\mathrm{Im}(h(u)) = \mathrm{Im}(h(\pm i)) = 0$ corresponds to the equation:

$$x(x^2 - 3y^2 + 3) = 0\ .$$

From this we get the following graph for the paths of steepest descent.



Here as in Case I the arrows point in the direction of steepest descent. Now we see that our path of integration must be:



The rest of the computation is carried out by standard methods [13]. My result was:

(A.4.26) $I_D \sim$

$$\frac{e^{-\frac{2\beta'}{3}}}{2\pi} \left| \sum_{n=0}^{\infty} \frac{(-1)^n \, \Gamma(\frac{6n+1}{2})}{(2n)!\, 3^{2n} \beta'^{\, n+1/2}} - \frac{1}{\Gamma(\frac{D+2}{2})} \sum_{n=0}^{\infty} \frac{\Gamma(\frac{2n+3}{2})(-1)^n A^D_{2n+1}}{\beta'^{\, n+3/2}} \right.$$

whereas in Case I

$$A_n^D = \sum_{k=0}^{n} \frac{\Gamma(\frac{3n-3k+1}{2})}{(n-k)!\, 3^{n-k}\, \Gamma(\frac{n-k+1}{2})} \sum_{\ell=0}^{k} \frac{\Gamma(\frac{2\ell+k+1}{2})\, \Gamma(k-\ell+2+\frac{D}{2})}{(k+1)!\ \Gamma(\frac{k+1}{2})\ 3^{\ell}} \binom{k}{\ell}$$

$$\beta' = \frac{[2m(V(\underset{\sim}{r})-E)]^{3/2}}{m\hbar\ |\underset{\sim}{\nabla} V|}$$

From (A.4.23) and (A.4.25):

$$\text{(A.4.27)} \quad \rho(\underset{\sim}{r}) = \frac{\Gamma(\frac{D}{2})\, \Omega_D}{h^D} \left[ \frac{2m(V(\underset{\sim}{r})-E)}{\beta'} \right]^{D/2} \cdot I_D$$

and from (A.4.24) and (A.4.25)

$$\text{(A.4.28)} \quad t(\underset{\sim}{r}) = \frac{\Gamma(\frac{D+2}{2})\, \Omega_D}{2m\ h^D} \left[ \frac{2m(V(\underset{\sim}{r})-E)}{\beta'} \right]^{\frac{D+2}{2}} I_{D+2}$$

# References

[1] Dirac, P.A.M., Proc. Cambridge Phil. Soc. 26 376 (1930)

[2] Weizsäcker, C.F. von, Z. Physik 96 431 (1935).

[3] Kompaneets, A. S. and Pavlovskii, E. S., Soviet Phys. JETP 31(4) 328 (1957).

[4] Kirzhnits, D. A., Soviet Phys. JETP 32(5) 64 (1957).

[5] Golden, S., Phys. Rev. 107 1283 (1957).

[6] Macke, Von W. and Rennert, P., Ann. der Physik 12 84 (1963).

[7] Kohn, W. and Sham, L. J., Phys. Rev. 137 A1697 (1965).

[8] Bethe, Hans A., Intermediate Quantum Mechanics (New York, W. A. Benjamin, Inc., 1964).

[9] Baraff, G. A., and Borowitz, S., Phys. Rev. 121 1704 (1961).

[10] E. Wigner, Phys. Rev. 40, 749(1932).

[11] J. E. Moyal, Proc. Cambridge Philos. Soc. 45, 99 (1949).

[12] J. G. Kirkwood, Phys. Rev. 44, 31 (1933).

[13] A. Erdélyi, Asymptotic Expansions (Dover Publications, Inc. 1956).

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

NYU
NYO-
1480-75 Percus c.1

The one body Wigner-Moyal

NYU
NYO-
1480-75 Percus c.1
AUTHOR
The one body Wigner-Moyal
TITLE
density...

| DATE DUE | BORROWER'S NAME |
|---|---|
| | |
| | |
| | |
| | |

N.Y.U. Courant Institute of
Mathematical Sciences
251 Mercer St.
New York, N. Y. 10012

AUG 4 1967

DATE DUE

| | | | |
|---|---|---|---|
| | | | |

GAYLORD PRINTED IN U. S. A.